

Implementation of Booth Models for Fission Product Release in SIRIUS Code

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1. Introduction

CINEMA code is an integral severe accident analysis code system composed of CSPACE for in-vessel phenomena, SACAP for ex-vessel phenomena, SIRIUS for fission product (FP) behavior, and a MASTER module that exchanges data between the codes at each time step [1,2]. For FP release from fuel, SIRIUS code has conventionally used CORSOR, CORSOR-M, and CORSOR-O models. These empirical models calculate the instantaneous fractional release rate mainly from the current fuel temperature and the remaining inventory.

In contrast, the Booth model calculates FP release based on diffusion within an equivalent spherical UO₂ grain [3]. The temperature-dependent diffusion coefficient is accumulated in a dimensionless state, Theta. Therefore, FP release depends not only on the current fuel temperature but also on the previous temperature history and the grain radius. Even at the same current temperature and remaining mass, two nodes can have different releases when their previous temperature histories are different.

Table I. Fundamental difference between CORSOR and Booth release models [3,4]

Item	CORSOR models	Booth models
Concept	Empirical release-rate correlation	Grain-interior diffusion
Driving quantity	Current temperature T	Accumulated diffusion state Θ
History	No diffusion state	$\Theta = \int D/a^2 dt$
Grain radius	Not explicit	Sets diffusion time scale
Species/class	Empirical rate coefficients	Class D_k or Cs-based scaling
Relocation	No diffusion history to move	History follows relocating fuel

This difference also requires a different calculation structure in SIRIUS code. The Booth model requires a diffusion-history variable that is continuously preserved. CORSOR-Booth and Revised CORSOR-Booth additionally require gas-side mass-transfer properties. Therefore, Booth models are implemented as separate fuel-release calculation paths, while the existing SIRIUS source, transport, phase-change, and deposition calculations are retained.

A similar calculation structure is used in MELCOR. CORSOR-type empirical release models and Booth-type models use different calculation routines and state variables [5-8]. This structure was used only as a reference for implementing the Booth calculation paths in SIRIUS code.

In this study, five Booth-based FP release models were implemented in SIRIUS code: CORSOR-Booth, ORNL-Booth, Modified ORNL-Booth, Revised CORSOR-Booth, and New ORNL-Booth. Their development

relationship is shown in Fig. 1. The five models use the same Original Booth grain-diffusion basis, but differ in the diffusion-history variable, the location of the radionuclide-class coefficient, and the treatment of gas-side resistance [3-8].

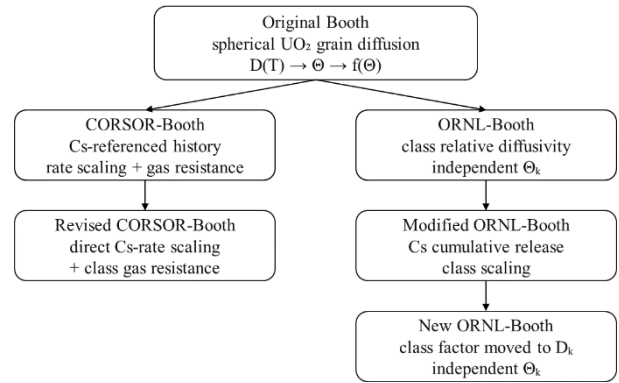


Fig. 1. Development genealogy of the Booth-based models.

2. Theoretical Basis and Model Evolution

2.1 Common grain-diffusion kernel

For a spherical grain with radius a , uniform initial concentration, and a perfect-sink surface, the Booth model is based on the following Fick diffusion equation [3].

$$\frac{\partial C}{\partial t} = \frac{D(T)}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial C}{\partial r} \right) \quad (1)$$

$$C(a, t) = 0 \quad (2)$$

$$\left. \frac{\partial C}{\partial r} \right|_{r=0} = 0 \quad (3)$$

$$C(r, 0) = C_0 \quad (4)$$

At the perfect-sink boundary, an FP reaching the grain surface is assumed to be immediately released from the grain. Therefore, the analytical solution represents the diffusion limitation inside the grain. The effective grain radius a , rather than the pellet radius, determines the characteristic diffusion time scale a^2/D .

The diffusion coefficient depends on fuel temperature according to the Arrhenius relation, and the diffusion progress is accumulated as follows [4,6].

$$D_k(T) = D_{0,k} \exp \left(-\frac{Q_k}{RT} \right) \quad (5)$$

$$\theta_{k,n+1} = \theta_{k,n} + \frac{D_k(T_n) \Delta t}{a_k^2} \quad (6)$$

In continuous form, $\theta_k = \int D_k[T(t)]/a_k^2 dt$. Therefore, θ represents the accumulated diffusion history according to fuel temperature. A short period at high temperature can increase the diffusion history more than a much longer period at low temperature.

As shown in Eqs. (5) and (6), $\Delta\theta$ is proportional to $D(T)\Delta t/a^2$. Therefore, higher fuel temperature increases the diffusion coefficient, while a smaller grain radius increases the diffusion progress. For example, reducing a by half increases $\Delta\theta$ by a factor of four at the same T and Δt [3,4].

For the spherical perfect-sink problem, the exact cumulative fraction released from the initial grain inventory is given by Eq. (7) [3].

$$f_k(\theta) = 1 - \frac{6}{\pi^2} \sum_{n=1}^{\infty} \frac{\exp(-n^2\pi^2\theta)}{n^2} \quad (7)$$

The value of Eq. (7) is a cumulative released fraction, not an instantaneous release rate. When the infinite series is directly truncated, a small artificial release can remain at $\theta = 0$. To avoid this numerical error, the current evaluator uses the short-time approximation for $\theta < 1.0 \times 10^{-3}$ and at least 100 series terms above this range. These values are numerical settings and not Booth model coefficients.

ORNL provides the following two-region approximation [4].

$$f(\theta) = \begin{cases} 6\sqrt{\theta/\pi} - 3\theta, & \theta < 0.1547 \\ 1 - \frac{6}{\pi^2} \exp(-\pi^2\theta), & \theta \geq 0.1547 \end{cases} \quad (8)$$

The first branch represents the short-time square-root diffusion region, and the second branch uses the $n = 1$ long-time term of Eq. (7). Since f is a cumulative released fraction, the release fraction applied to the remaining inventory during each time step is

As θ approaches zero, f also approaches zero according to the square-root diffusion behavior. As θ increases, f approaches unity and the $n = 1$ exponential term becomes dominant. Therefore, the transition values in the piecewise equations are numerical criteria for evaluating the same diffusion solution and do not represent a physical transition [3,4].

$$f_{\text{step}} = \frac{f_{\text{new}} - f_{\text{old}}}{1 - f_{\text{old}}} \quad (9)$$

$$0 \leq f_{\text{step}} \leq 1 \quad (10)$$

CORSOR-Booth and Revised CORSOR-Booth use the CORSOR-specific transition value $\theta = 1/\pi^2$, while the ORNL-based models use 0.1547 [4-6].

2.2 Model-specific formulations

The number of diffusion-history variables required for each model depends on where the class coefficient is applied. CORSOR-Booth, Modified ORNL-Booth, and Revised CORSOR-Booth first calculate the Cs diffusion history and then apply scaling to the other classes. Therefore, one Cs diffusion-history variable is required for each node. In ORNL-Booth and New ORNL-Booth, the class coefficient is applied to D_k before integration, and each class requires an independent θ_k [4,7,8].

CORSOR-Booth first calculates the Booth release of Cs. The Cs cumulative release increment is converted to a release rate based on the remaining inventory. The Cs gas-side resistance is then removed, the class factor S_k is applied to the solid-side rate, and the class gas-side resistance is added again [5,6].

$$\text{DIFF}_{\text{Cs}} = \left(\frac{1}{\text{ReleaseRate}_{\text{Cs}}} - \frac{1}{\text{Rate}_{\text{gas,Cs}}} \right)^{-1} \quad (11)$$

$$\text{DIFF}_k = S_k \text{DIFF}_{\text{Cs}} \quad (12)$$

$$\text{Rate}_{\text{tot},k} = \left(\frac{1}{\text{DIFF}_k} + \frac{1}{\text{Rate}_{\text{gas},k}} \right)^{-1} \quad (13)$$

The inverse calculation is not defined when $\frac{1}{\text{ReleaseRate}_{\text{Cs}}} - \frac{1}{\text{Rate}_{\text{gas,Cs}}} \leq 0$. Therefore, this condition is explicitly checked in the current implementation. This inverse calculation of the Cs gas-side resistance is the main difference between CORSOR-Booth and Revised CORSOR-Booth.

ORNL-Booth uses the class data as relative diffusion coefficients. Therefore, each class has an independent D_k and θ_k [4].

$$D_k(T) = R_{D,k} (1.0 \times 10^{-6}) \exp\left(-\frac{45779}{T}\right) [\text{m}^2/\text{s}] \quad (14)$$

Since $R_{D,k}$ is applied to the diffusion coefficient, it changes the diffusion progress throughout the transient. Therefore, classes with low relative diffusivity show delayed release. Gas-side mass-transfer resistance is not included in the original ORNL-Booth model.

Modified ORNL-Booth uses one Cs diffusion history and applies the adjusted class coefficient to the cumulative remaining fraction [5,7]. The resulting relation is

$$1 - f_k = (1 - f_{\text{Cs}})^{S_k} \quad (15)$$

For a small released fraction, $f_k \approx S_k f_{\text{Cs}}$. Revised CORSOR-Booth uses a separate Cs-based calculation path and does not perform the inverse Cs gas-resistance calculation of CORSOR-Booth. Instead, it uses

$$\text{DIFF}_k = S_k \text{ReleaseRate}_{\text{Cs}} \quad (16)$$

The class gas-side resistance is then combined using Eq. (13) [7]. Therefore, Modified ORNL-Booth and Revised CORSOR-Booth can use the same adjusted class coefficients, but their calculation procedures are different.

New ORNL-Booth applies the adjusted class factor to the diffusion coefficient instead of the cumulative released fraction or release rate [7,8].

$$D_k(T) = S_k D_0 \exp\left(-\frac{Q}{RT}\right) \quad (17)$$

$$\theta_{k,n+1} = \theta_{k,n} + \frac{D_k(T_n) \Delta t}{a^2} \quad (18)$$

This change is not mathematically equivalent to Eq. (15). For small θ , Modified ORNL-Booth gives $f_k \approx S_k f_{Cs}$, while Eqs. (17) and (18) give $f_k \approx \sqrt{S_k} f_{Cs}$ for New ORNL-Booth. For $S_k = 4.0 \times 10^{-4}$, the initial scaling differs by approximately a factor of 50. The published New ORNL-Booth data do not provide a U class coefficient. Therefore, U release is not calculated using a coefficient taken from another model.

The main differences among the five Booth-based models are the diffusion-history variable, the location of the class coefficient, the treatment of gas-side mass-transfer resistance, and the method used to convert the cumulative Booth result to the current-step release.

Table II. Core mathematical distinctions among Booth models

Model	History	Class coefficient applied to	Gas-side
CORSOR-Booth	θ_{Cs}	Solid-side diffusion rate	Included
ORNL-Booth	θ_k	Diffusion coefficient D_k	Not in original
Modified ORNL-Booth	θ_{Cs}	Cumulative release fraction f_k	Not used
Revised CORSOR-Booth	θ_{Cs}	Solid-side diffusion rate	Included
New ORNL-Booth	θ_k	Diffusion coefficient D_k	Not used

CORSOR-Booth uses $D_0 = 2.5 \times 10^{-7} \text{ m}^2/\text{s}$, $Q = 3.814 \times 10^5 \text{ J/mol}$, and $a = 6.0 \text{ } \mu\text{m}$. ORNL-Booth uses the original $45779/T$ exponent reported in the ORNL model. Modified ORNL-Booth and Revised CORSOR-Booth use the adjusted parameter set reported in the later assessments. New ORNL-Booth uses the published adjusted class diffusion factors, while the same grain radius is retained in the present SIRIUS implementation [5-8].

3. Implementation in SIRIUS

SIRIUS code implements the five Booth models (CORSOR-Booth, ORNL-Booth, Modified ORNL-Booth, Revised CORSOR-Booth, and New ORNL-Booth) as separate FP release branches. The existing SIRIUS source and transport calculations after fuel release are used without changing the basic calculation structure.

3.1 Preservation of diffusion history during fuel relocation

CORSOR-Booth, Modified ORNL-Booth, and Revised CORSOR-Booth store θ_{Cs} for each node. ORNL-Booth and New ORNL-Booth store $\theta_{group}[k]$ for each node and FP group. Since θ represents the accumulated diffusion history of the fuel, this history must also move when UO_2 is relocated. SIRIUS code therefore transports the following mass-weighted history variables.

$$H_{Cs} = M_{\text{UO}_2} \theta_{Cs} \quad (19)$$

$$H_k = M_{\text{UO}_2} \theta_k \quad (20)$$

$$\theta = \frac{H}{M_{\text{UO}_2}} \quad (21)$$

The same UO_2 relocation fraction used for the in-fuel FP inventory is applied to these history variables. After relocation, θ is reconstructed using Eq. (21). This method preserves the Booth history without changing the current lumped-node structure. However, because $f(\theta)$ is nonlinear, mass-weighted mixing is an approximation when fuel with different diffusion histories is mixed in one node.

3.2 Gas-side closure for the CORSOR branches

For CORSOR-Booth and Revised CORSOR-Booth, the gas-side mass-transfer rate is calculated as follows.

$$\text{Rate}_{\text{gas},k} = A_{\text{fuel}} \frac{Nu D_{\text{gas},k}}{d_{\text{fuel}}} \frac{P_{\text{eq},k}}{R T_{\text{fuel}}} \quad (22)$$

Gas density, viscosity, heat capacity, thermal conductivity, velocity, pressure, and hydraulic diameter are obtained from the coupled thermal-hydraulic calculation. The current model uses $Re = \frac{\rho_g |v_g| D_h}{\mu_g}$, $Pr = \frac{\mu_g c_p}{k_g}$, $Nu = 4.36$ for $Re < 10000$, and $Nu = 0.023 Re^{0.8} Pr^{0.4}$ otherwise. The gas diffusion coefficient $D_{\text{gas},k}$ is calculated by the Chapman-Enskog equation using the existing SIRIUS Lennard-Jones data, and the equilibrium vapor pressure $P_{\text{eq},k}$ is calculated using the existing saturation-pressure data. The published CORSOR-Booth equation also includes a free-stream FP concentration term [5,6]. This back-pressure term is not included in Eq. (22) in the present implementation.

4. Preliminary Verification

Before coupled transient calculations, standalone calculations were performed to confirm the equations and implementation. For $T = 2000 \text{ K}$, $\Delta t = 1000 \text{ s}$, $a = 6 \text{ } \mu\text{m}$, and $\theta_0 = 0$, the cumulative Cs releases were 18.145% for ORNL-Booth and 17.750% for Modified ORNL-Booth, Revised CORSOR-Booth without gas resistance, and New ORNL-Booth. The

corresponding Mo releases were 4.715%, 3.833%, 3.833%, and 8.163%, and the Ru releases were 0.382%, 0.049%, 0.049%, and 0.931%, respectively. These results show the expected differences caused by the locations of the class coefficients in Eqs. (14)-(18).

A parameter sweep for $T = 500\text{--}3500\text{ K}$ and $\Delta t = 1.0 \times 10^{-6}\text{--}1000\text{ s}$ showed no errors. θ increased monotonically, and the cumulative released fractions remained between 0 and 1. The time-step release fraction based on the remaining inventory agreed with the cumulative solution. The inverse and recombination of the CORSOR-Booth resistances were also confirmed.

5. Conclusion

Five Booth-based FP release models were implemented in SIRIUS code as separate options. The models share the same spherical grain-diffusion basis but use different diffusion-history variables, class-coefficient locations, and gas-side resistance treatments.

The existing SIRIUS species/group source and transport calculations were retained, and the Booth diffusion history was transferred with relocated UO₂. The standalone calculations confirmed the basic equations and numerical behavior. Further coupled transient calculations and comparisons with FP release experiments will be performed in future work.

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