

# Using Calibrated Water Data for Preliminary Validation of the SRT Code for Advanced Reactors

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prepared by

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IAEA International Conference on Topical Issues in Nuclear Installation Safety  
October 18-21, 2022  
Vienna, Austria

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# USING CALIBRATED WATER DATA FOR PRELIMINARY VALIDATION OF THE SRT CODE FOR ADVANCED REACTORS

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## Abstract

Recent interest and corresponding progress worldwide regarding advanced nuclear reactors has renewed focus on their performance and related safety assessments. Specifically, the U.S. Nuclear Regulatory Commission has emphasized the importance of mechanistic approaches to source term analysis for advanced reactor licensing applications, which attempt to realistically account radionuclide transport and retention phenomena. Further model development is required due to the numerous and complex physical and chemical phenomena associated with mechanistic source term analyses. Reflecting the need for modeling advancement, Argonne National Laboratory developed a mechanistic source term analysis tool for sodium fast reactors. The Simplified Radionuclide Transport (SRT) code describes fuel pin failure (for simulating the initial condition at the point of fuel pin breach), bubble scrubbing, deposition, leakage and following environmental impact. In the current work, a validation study of the SRT bubble scrubbing model is performed using a water-loop experiment performed at the University of Wisconsin-Madison. Through the analysis, the approach and fundamental bubble scrubbing models in SRT, which examine the removal of aerosols within the bubble as it is transported through a pool, have been widely evaluated. The results of the assessment demonstrate a high level of agreement in the regions of greater aerosol size. In the parameter range of minimal aerosol removal, the simulation slightly underpredicts the experiment results; however, considering the scale of plots and huge uncertainties inherently included, the deviation can be judged to be minor and would produce a conservative result. In addition, uncertainty analysis has been further refined to reflect the experimental distribution of parameters including aerosol sizes, which induces a span of performance for each representative aerosol size. Based upon the initial validation results along with uncertainty effects, SRT is expected to provide meaningful insights for the analysis of bubble scrubbing. Future sodium-loop tests will provide further validation basis.

## 1. INTRODUCTION

With worldwide emphasis on climate change due to looming catastrophic symptoms, nuclear power is a promising option for the future. Along with the need for an increase of nuclear energy, reactor design is shifting to include inherent and passive safety. Included in this category, advanced types of reactors are being considered and corresponding regulatory/licensing approaches are actively being developed, especially in United States. As part of this movement, the U.S. Nuclear Regulatory Commission (USNRC) has stated an expectation for a mechanistic source term analysis as a crucial part of the licensing process [1, 2]. As protection of the public and the environment is the primary concern of licensing, the source term analysis is central to the safety basis. Reflecting the urgent needs of the advanced reactor community, Argonne National Laboratory (Argonne) developed a simulation tool for the mechanistic source term analysis of sodium-cooled fast reactors (SFRs) and microreactors. The Simplified Radionuclide Transport (SRT) code can simulate the transport and retention of radionuclides over multiple phenomena, including fuel pin failure (for the initial condition before the release of radionuclides into the coolant or gas), bubble scrubbing, vaporization, deposition, leakage and environmental impacts. The code also tracks the decay phenomenon of nuclides during the transport process.

As highlighted in preceding reports [3, 4], the source term phenomena associated with potential SFR transient scenarios are complex. In particular, aerosols ejected from failed fuel pins may enter the sodium pool encapsulated inside gas bubbles and can potentially bypass retention within the sodium pool. Therefore, bubble transport of radionuclide aerosols has been identified as a top priority for model validation [4]. The degree of aerosol removal during the bubble transport process is described in terms of decontamination factor (DF), a ratio between the initial amount of released aerosols to the amount after escaping the pool. The current work examines a recent validation effort of the SRT code and the calculation of the DF utilizing experimental data.

### 1.1. Calibrated water data and SRT code

The current study focuses on validation of the SRT code utilizing bubble transport data from a water-loop experiment performed at the University of Wisconsin Madison (UW) [5]. Sodium loop tests are also planned, but a water-loop experimental series was conducted first, as a proof of concept. Fortunately, the models within SRT are applicable to multiple working fluids, with proper modifications to the fluid properties within the code. For the purpose of this work, only the bubble scrubbing module of SRT was utilized. As described in ref [6], the bubble scrubbing model in SRT examines aerosol removal during bubble rise inside the pool. Several mechanisms are incorporated in the model to mechanistically simulate the phenomenon based on Powers and Sprung [7]: Brownian diffusion, inertial impaction, gravitational sedimentation and condensation, which are described further in Section 1.2. The condensation term is not considered in this study, as the carrier gas was air and the target experimental data was acquired at room temperature condition.

A summary of experimental conditions is shown in TABLE 1, where an overview of the parameters varied during the experimental series is provided. As highlighted, the experimental campaign sought to be comprehensive in respect to parameters such as aerosol diameter/density/concentration, along with bubble diameter and pool depth.

TABLE 1. PARAMETRIC CONDITIONS CONSIDERED IN THE EXPERIMENT

Parameter	Unit	Value
Aerosol mean diameter	$\mu\text{m}$	0.018 – 18
Aerosol density	$\text{g/cm}^3$	2.7 / 8.9
Aerosol concentration	$\text{g/m}^3$	26.5 / 13.2
Bubble effective diameter	cm	1.81 / 2.19 / 2.87 / 3.27
Pool depth	ft	6 / 3

### 1.2. SRT mechanisms and basics

Brownian diffusion describes particle diffusion inside bubbles and is described in terms of environmental temperature, bubble shape/property and rise velocity. The term tends to decrease with increasing size of the aerosol. A coefficient for the aerosol removal ( $\alpha_D$ ) is expressed as follow (variable nomenclature is provided at the end of the article):

$$\alpha_D = \sqrt{\frac{288\theta}{\pi U_B D_B^3}} \left[ \frac{(E^2 - 1)F}{1 + \sqrt{4 + 2(E^2 - 1)}} \right]$$

where,

$$\begin{aligned} \theta &= \frac{k_B T_B C_n}{3\pi\mu_B d_a} \\ C_n &= 1 + \frac{2\lambda}{d_a} \left[ 1.257 + 0.4e^{-0.55\frac{d_a}{\lambda}} \right] \\ \lambda &= \frac{k_B T_B}{\sqrt{2}\pi d_{B,mol}^2 P_B} \\ F &= \left[ \frac{1.76E^2}{E^2 - 1} - \sqrt{2} \right]^{1/2} \left[ \frac{E^2 \tan^{-1} \sqrt{E^2 - 1}}{\sqrt{E^2 - 1}} - 1 \right]^{-1/2} \end{aligned}$$

The coefficient in the exponential term of Brownian diffusion requires a limiting condition when the bubble shape approaches spherical (as the denominator approaches zero). Small-sized bubbles tend to form spherical shape with unity of eccentricity.

$$\alpha_D = 1.83 \sqrt{\frac{8\theta}{\pi U_B D_B^3}}$$

The inertial impaction causes direct removal of aerosols by inertial movement of aerosols inside bubbles. The term is strongly dependent on bubble geometry and aerosol size, and it becomes a dominant factor as aerosol size increases. The coefficient for the inertial impaction is described as follow:

$$\alpha_I = \frac{6U_B\tau G}{D_B^2}$$

where,

$$\tau = \frac{\rho_a d_a^2 C_n}{18\mu_B}$$

$$G = \frac{E^{4/3}[(E^2 - 1)^2 + (E^2 - 1)^{3/2}(E^2 - 2)\tan^{-1}\sqrt{E^2 - 1}]}{[\sqrt{E^2 - 1} - E^2\tan^{-1}\sqrt{E^2 - 1}]^2}$$

As for the Brownian diffusion, the inertial impaction also requires a limiting condition when the bubble shape becomes spherical, where the eccentricity approaches to unity. The form can be denoted as follow:

$$\alpha_I = \frac{18U_B\tau}{D_B^2}$$

The gravitational sedimentation describes the removal of aerosol particles by the gravitational force. The term is related to bubble shape, gravitational acceleration, and aerosol particle density. As with the previous inertial impaction term, the gravitation sedimentation provides a continuously increasing contribution to the decontamination process with increasing aerosol size. The coefficient used for the gravitational sedimentation is summarized below:

$$\alpha_G = \frac{1.5g\tau E^{2/3}}{D_B U_B}$$

The eccentricity used in each mechanism is determined based on the Tadaki number ( $Ta$ ), that consists of bubble Reynolds number and Morton number, as below:

$E = 1$	$Ta \leq 1$
$E = 1/[0.81 + 0.206 \times \tanh\{2 \times (0.8 - \log_{10} Ta)\}]^3$	$1 < Ta \leq 39.8$
$E = 4.167$	$Ta > 39.8$

It was further assumed that the coefficients do not change as the bubble rises due to negligible impact of local hydraulic pressure change, which means all consisting parameters like bubble size and rise velocity are determined and fixed from the bubble release location (constant values). With the simplified assumption, the decontamination factor for each mechanism can be described in exponential forms, where initial release depth is directly multiplied to the exponential term. The total decontamination factor can be finally expressed by the multiplication of each consisting mechanism:

$$DF_D = e^{\alpha_D H_{pool}} \quad DF_I = e^{\alpha_I H_{pool}} \quad DF_G = e^{\alpha_G H_{pool}}$$

$$DF = DF_D DF_I DF_G$$

SRT does not consider thermophoresis or diffusiophoresis, as it assumes complete equilibrium during the scrubbing process, and the code does not include interaction between aerosol particles (such as particle growth), nor models for bubble dynamics such as bubble interaction and jet regime. However, multiple options for bubble rise velocity that provide crucial impact to the decontamination performance have been considered in SRT, which are applicable to a wide range of bubble environments. Some options divide bubble regime into further detail, dependent upon bubble effective diameter, and provide a rise velocity correlation of bubble for each regime. For

a single bubble condition, the bubble region criterion by Wallis [8] has been used in this study to account for various bubble shapes (TABLE 2). For bubble swarm condition, correlations suggested by Ramsdale et al. [9], and Owczarski and Burk [10] have been further considered through the user-defined function in SRT.

TABLE 2. WALLIS BUBBLE REGIME CORRELATION

Region	Dimensionless speed	Value
Region 1	$U^*=r^{*3}/3$	$r^*<1.5$ and $U^*<0.75$
Region 2A	$U^*=0.408r^{*1.5}$	$1.5<r^*<13.4$ and $0.75<U^*<20$
Region 2D	$U^*=r^{*2}/9$ or $U^*=C_0r^{*2}$ ( $C_0<1/9$ )	$13.4<r^*$ and $20<U^*$
Region 3	$U^*=\sqrt{2}r^{*1/2}P^{1/6}$	Between the “fluid sphere” lines and $U^{*2}=2r^*$
Region 4	$U^*=\sqrt{2}P^{1/12}$	Between the “solid sphere” lines and Region 5
Region 5	$U^*=r^{*1/2}$	Only for bubbles

— Swarm rise velocity correlations

- GE-BUSCA Correlation

$$U_B = \sqrt{\frac{28 \alpha g Y}{30(1-\alpha)}}$$

$$Y = 0.65 D_{orf} \left[ \frac{Q_{swarm}}{\sqrt{g D_{orf}^5}} \right]^{2/5}$$

- Colder-BUSCA Correlation

$$U_B = 2.221 \sqrt{D_B} \left[ 1 - \alpha + \frac{\alpha^{1/3}}{\sqrt{D_B}} \left( \frac{Q_{swarm}}{0.5812} \right)^{1/5} \right]$$

- SPARC90 Correlation

$$U_B = 5E - 3 \times \sqrt{\frac{Q_{swarm} \times 1E3 + 5.33}{3.011E - 3}} \left[ 2 - 3.975E - 2 \times \frac{H_{pool}}{2} \right]$$

(Based on average velocity with respect to pool depth)

Uncertainty information of each major parameter has been considered for the simulation using SRT, and corresponding random DF values have been derived by performing 10,000 samples for the parameters within a given confidence level (95 percentile). The uncertainty analysis has been performed for the single bubble case only as given uncertainty value of bubble size approaches to the mean value itself for the swarm condition, which induces a huge relative scale of uncertainty, leading to unrealistic results. Also, SRT can describe skewed uncertainty distributions in positive and negative directions from the mean value, and each directional uncertainty information has been implanted reflecting real parametric uncertainty distribution. Based on the span of DF distribution, mean of the distribution has been derived.

## 2. COMPARISON RESULT AND DISCUSSION

### 2.1. Bubble size effect

Four sizes of bubbles were considered in the experiment procedure, and corresponding effective bubble diameters have been used in the SRT simulation. As can be observed in Fig. 1, where mean values of parameters are used for the reference cases, DF values steadily decrease with increasing bubble size for the whole range of aerosol sizes considered in this study. The surface area per volume decreases with increasing bubble diameter, which degrades the interaction interface. The prediction results show agreeable trends with the experiment,

especially in the region of large aerosol sizes. In the most deteriorated region (the minimum DF range), SRT provides conservative trends; the difference could be treated to be minor considering the scale of plot and huge scatter in the area, where several orders differences are easily observed by sensitive and uncertain phenomena included.

Uncertainty information of parameters have been further considered to derive distribution of random DF values. Based on the span of DF values, mean of the distribution has been summarized in Fig. 2. The mean plot shows similar trends at large aerosols, while it starts to soar below certain aerosol sizes, due to increasing uncertainty and sensitiveness (observed through the log-scale of x-axis) at small-sized aerosol particles. Interestingly, the surging phenomenon predicts exceptionally well the experimental data. The mean trend still provides conservative prediction at the lowest performance region, where the capture efficiency against radionuclides is the lowest.

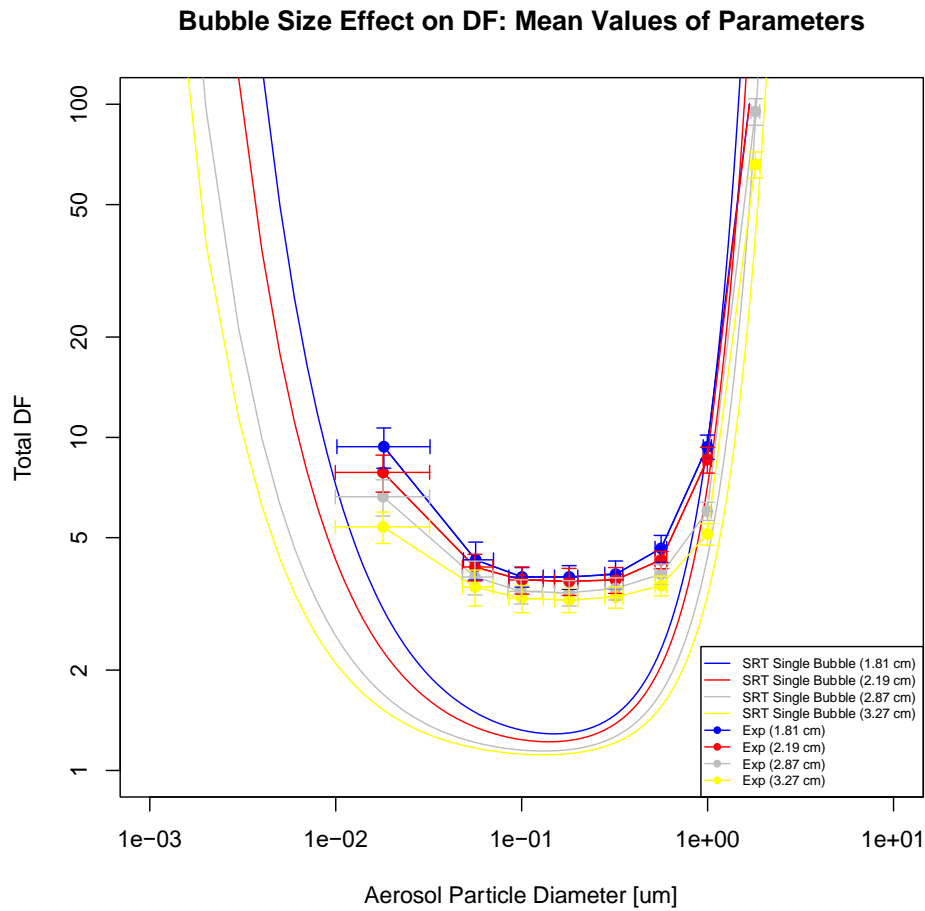


FIG. 1. Bubble size effect on DF trends using mean values of parameters (reference case).

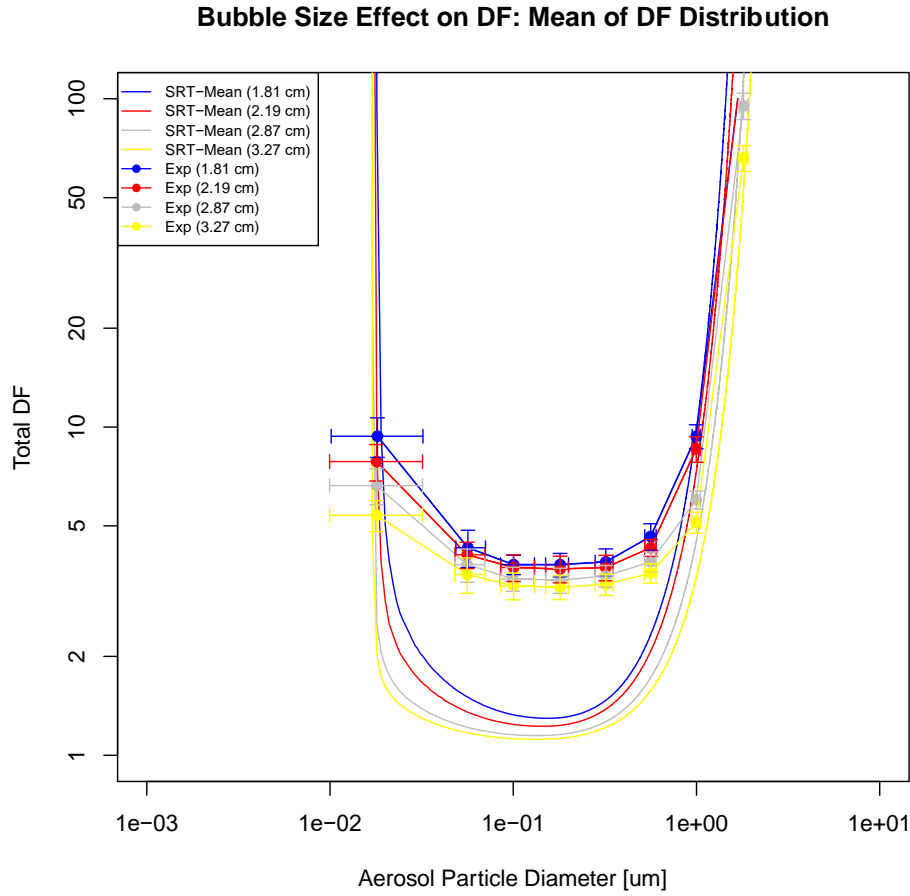


FIG. 2. Mean of DF distribution by uncertainty information.

## 2.2. Bubble swarm effect

To describe the bubble swarm condition, two types of bubble rise velocities (for a single bubble and swarm bubbles) have been considered for comparison. When the correlation for a single bubble rise velocity is adopted, the prediction result shows good agreement with the experimental data at both ends, while deviation in the most deteriorated region becomes increased compared with single bubble measurement in the previous section (Fig. 3). Still, the effect can be treated minor considering the log-scale of the plot and quite uncertain phenomena incorporated. By including several correlations for the bubble swarm, the prediction shows more discrepancies, especially at large aerosols (Fig. 4). According to the considered swarm correlations, the rise velocity is expected to increase compare with a single bubble correlation. Besides, contribution of the inertial impaction drastically increases with bubble rise velocity since the term is included in the coefficient as a proportional term. By this way, the difference in rise velocity for the swarm region shifts the minimum point, and thus, advances the rapidly increasing trend.



### Bubble Size Effect on DF with a Single Bubble Correlation

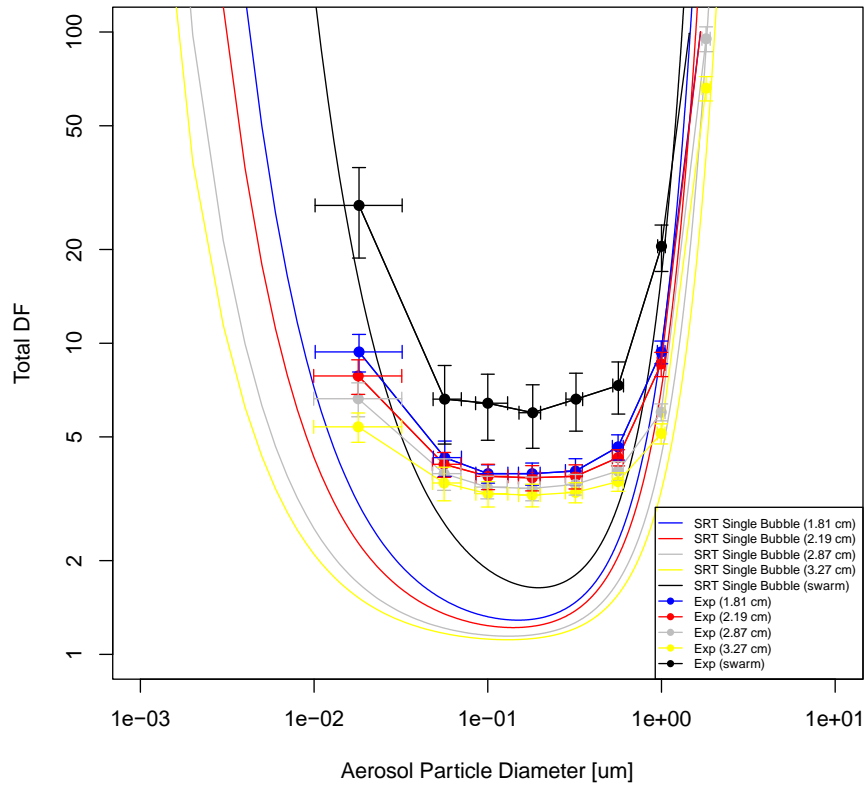


FIG. 3. DF prediction by a single bubble correlation.

### Bubble Swarm Effect on DF: Mean Values of Parameters

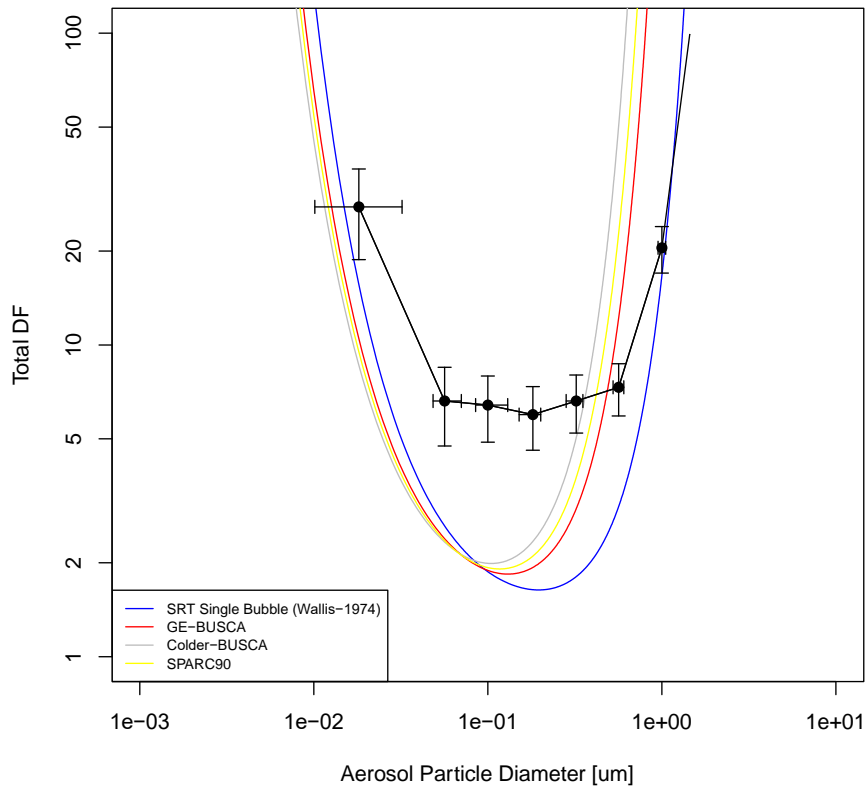


FIG. 4. DF for swarm bubbles using mean values of parameters (reference case)

### 3. CONCLUSION

Removal of radionuclide aerosols during transport in bubbles within the sodium pool is a key phenomenon for SFR mechanistic source term analyses. The bubble scrubbing model within SRT has been introduced and the results of a validation exercise based on an experimental water-loop are summarized. The bubble size and swarm effect are assessed along with uncertainty analysis. A correlation for a single bubble velocity has been adopted for the bubble size effect, while several additional correlations suggested for the swarm condition in preceding documents have further been considered in the swarm condition. According to the results, bubble geometry and corresponding rise velocity have crucial impacts on the overall trends, observed from both prediction and measured data. The decontamination performance tends to decrease with increasing bubble size both in the prediction and measurement, due to decreased surface area to volume ratio. The prediction shows exceptionally agreeable result especially at large aerosols, while it underpredicts at the lowest performance region. However, the deviation seems marginal considering the plot scale (log-scale) and inherent huge uncertainty of the phenomenon. For the swarm condition, the prediction still holds the overall trends with slight growth of the discrepancy at the lowest performance region, but the difference is still marginal. Also, considering the degraded decontamination at the region (the most severe condition in respect to radionuclide release), such conservative predictability is proper for practical purposes. Besides, the removal performance decrease and increase again with increasing aerosol size, due to change of major contributing mechanisms from Brownian diffusion into inertial impaction and gravitational settlement. Due to difference in each mechanism's formula, change of bubble rise velocity correlation in the swarm environment causes drastic effect especially at large aerosols.

Uncertainty information of each consisting parameter has been used for the uncertainty assessment in the single bubble case, and mean of DF distribution rapidly increases at conditions of great uncertainty (especially for small-sized aerosol particles), because of increasing uncertainty along with great sensitiveness by the aerosol size in the small-sized region. Besides, mean of DF distribution well predicts the measured data at both ends. According to the assessment, SRT shows agreeable results overall considering intrinsic complex phenomena and huge uncertainty included, which generally causes great discrepancies.

### 4. NOMENCLATURE

$\alpha_D$	= Removal coefficient for Brownian diffusion
$\alpha_I$	= Removal coefficient for Inertial impaction
$\alpha_G$	= Removal coefficient for Gravitational sedimentation
$\alpha$	= Swarm void fraction ('0.5' in this study based on [9])
$U_B$	= Bubble rise velocity
$D_B$	= Effective bubble diameter
$D_{orf}$	= Orifice diameter
$T_B$	= Gas temperature
$P_B$	= Gas pressure
$\mu_B$	= Gas dynamic viscosity
$d_{B,mol}$	= Effective diameter of gas molecules
$d_a$	= Aerosol diameter
$\rho_a$	= Aerosol density
$k_B$	= Boltzmann constant
$E$	= Eccentricity
$C_n$	= Cunningham factor
$g$	= Gravitational acceleration
$DF$	= Decontamination factor
$Q_{swarm}$	= Swarm volumetric flowrate
$H_{pool}$	= Pool depth

## ACKNOWLEDGEMENTS

The submitted manuscript has been created by UChicago Argonne, LLC, Operator of Argonne National Laboratory (“Argonne”). Argonne, a U.S. Department of Energy Office of Science laboratory, is operated under Contract No. DE-AC02-06CH11357. Argonne National Laboratory’s work was supported by the U.S. Department of Energy, Office of Nuclear Energy under contract DE-AC02-06CH11357.

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