

A Phenomenological Model for the Transport and Plugging of Aerosol Through Stress Corrosion Cracks

Spent Fuel and Waste Disposition

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SUMMARY

This report documents work performed under the Spent Fuel and Waste Disposition Campaign for the US Department of Energy Office of Nuclear Energy. This work was performed to fulfill the Level 3 milestone M3SF-20OR010207031 “Development and validation of phenomenological model on aerosol transport and plugging through stress corrosion cracks” within work package SF-20OR01020703 “Stress Corrosion Cracking - ORNL.”

Recent experimental evidence from Sandia (2018) demonstrated partial microchannel plugging due to particulate deposition. A direct consequence is that the accuracy of consequence assessments can be improved by accounting for the leak path deposition of aerosol in the source term. The filtration effect of microchannels, such as cracks, is relevant to the source term assessments. An important side effect of aerosol deposition in leak paths could be the plugging of the leak path.

This report summarizes current progress (as of end of FY19) on the development of a phenomenological model of aerosol transport, deposition, and plugging through microchannels. The purpose is to introduce a generic, reliable numerical model for prediction of aerosol transport, deposition, and plugging in leak paths that are similar to stress corrosion cracks while accounting for potential plugging formation. This effort includes (i) development of a numerical model to analyze the various deposition processes in leak paths and provide quantitative estimates of penetration factors, as well as an understanding of the variables that affect them, (ii) confirmation of model validity with theoretical and experimental data, and (iii) parametric analysis for different scenarios including various particle sizes, pressures, and crack dimensions. Such a model could be used to improve the accuracy of consequence assessments and reduce the uncertainty of radiological consequence predictive analyses by taking the filtering effect of leak path aerosol deposition and plugging into account in the source term.

This report includes: (i) an overview of main stress corrosion cracking characteristics, (ii) an overview of the developed numerical model to analyze the various deposition processes in leak paths, to provide quantitative estimates of penetration factors, and to gain an understanding of the variables that affect them, (iii) a summary of validation results and verification of the model’s validity with recent experimental results from Sandia and others, and (iv) a model application example.

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ACRONYMS

CISCC	chloride-induced stress corrosion cracking
CFR	US Code of Federal Regulations
DOE	US Department of Energy
DPC	dual-purpose canister
DSS	dry storage system
EPRI	Electric Power Research Institute
GDE	general dynamic equation
NWTRB	US Nuclear Waste Technical Review Board
ORNL	Oak Ridge National Laboratory
SCC	stress corrosion cracking

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SPENT FUEL AND WASTE DISPOSITION PROGRAM A PHENOMENOLOGICAL MODEL FOR THE TRANSPORT AND PLUGGING OF AEROSOL THROUGH STRESS CORROSION CRACKS

1. INTRODUCTION

Recent experimental evidence from Sandia (2018) demonstrated partial microchannel plugging due to particulate deposition. A direct consequence is that the accuracy of consequence assessments can be improved by accounting for the leak path deposition of aerosol in the source term. The filtration effect of such cracks is relevant to the source term assessments. An important side effect of aerosol deposition in leak paths could be the plugging of the leak path. Further research into this phenomenon is desirable.

1.1 Background

Modeling aerosol transport, retention, and plugging involves the thermal-hydraulic behavior of the canister and of the microchannel/crack, as well as the geometric characteristics of the microchannel/crack and the aerosol features. The minimum set of parameters that needs to be identified includes:

- **Thermo-hydraulics:** within this group, the most important parameters are the pressure inside the canister, gas composition, pressure drop and the wall temperature along the crack;
- **Crack geometry:** the parameters to be considered are mainly the crack path and its hydraulic diameter; information upon the crack section shape and curvature are also very important;
- **Aerosol features:** aerosol average composition, concentration and size distribution are the reference parameters, whilst others, regarding aerosol morphology, can be only taken with large uncertainties.

A compilation of available data in support of model development including (i) canister characteristics, e.g., pressure, temperature, heat load, environmental conditions, etc. (ii) particle size distribution within canister for various scenarios, (iii) crack characteristics, e.g., size, opening, roughness, etc., and (iv) past models and experiments involving aerosol transport can be found in [Chatzidakis, 2018a].

1.2 Modeling Capabilities

The proposed phenomenological model is based on the aerosol general dynamic equation and can simulate rough or smooth surfaces, irregular geometries, and unsteady flow. Four main deposition mechanisms—gravitational, Brownian diffusion, turbulent diffusion, and eddy impaction— have been included. Laminar, transition, and turbulent gas flow regimes have also been included in the model. The proposed model, currently under development, is being tested and compared with experimental and theoretical work to evaluate its validity and identify its range of applicability.

A wide range of particle size, distribution, pressure differential, flow regimes, and microchannel dimensions can be simulated using the current model. The model can predict pressure change over time due to depressurization (transient state) and particle deposition within a large vessel such as a canister, before, during, and following depressurization. A summary of the model characteristics is presented in Table 1. A summary of current validation status is shown in Table 2.

1.3 Purpose

This report outlines a generic phenomenological model of aerosol transport, deposition, and plugging through microchannels. It includes: (i) an overview of main stress corrosion cracking characteristics, (ii) an overview of the developed numerical model to analyze the various deposition processes in leak paths, to provide quantitative estimates of penetration factors, and to gain an understanding of the variables that affect them, (iii) a summary of validation results and verification of the model’s validity with recent experimental results from Sandia and others, and (iv) an application example.

Table 1. Summary of aerosol model capabilities.

Particle diameter	0.01 μm – 10 μm
Particle distribution	Monodisperse / Polydisperse
Pressure	4 Pa – 700 kPa
Microchannel dimensions	5 μm – 1 mm
Coagulation	Yes
Deposition mechanisms	Brownian, Gravitational, Turbulent, Inertial, Thermophoresis
Plugging	Yes
Steady state	Yes
Transient state	Yes
Flow regimes	Laminar, Transition, Turbulent
Depressurization	Yes
Fluid	Air, He

Table 2. Summary of aerosol tests in open literature and aerosol model validation status.

Experiment	Type	Material	ΔP	dp	D (or H \times W)	L	Validation status
Morton & Mitchell (1994)	Capillary	n/a	20–80 kPa	1–10 μm	28–35 μm	19–21 mm	Completed
Lewis (1995)	Slot	n/a	10 kPa	1–6 μm	100 $\mu\text{m} \times 40$ mm	n/a	Completed
Mosley et al. (2001)	Slot	Aluminum	2–20 Pa	0.05–5 μm	508 $\mu\text{m} \times 433$ mm	102 mm	Completed
Liu & Nazaroff (2003)	Slot	Concrete	4–10 Pa	0.02–7 μm	0.25 mm, 1 mm	4.5 cm	Completed
Gelain & Vendel (2007)	Crack	Concrete	0–12 kPa	0.8; 1.1; 4.1 μm	49.2 $\mu\text{m} \times 11.8$ m	0.1 m	Completed
Tian et al. (2017)	Capillary	Silica	60–450 kPa	<0.3 μm	5–20 μm	10–80 mm	Completed
Lai et al. (2012)	Slot	Aluminum	2–8 Pa	20–500 nm	50 mm \times 250 mm	90 mm	Completed
Nelson & Johnson (1975)	Capillary	n/a	3 kPa	3–5 μm	520 μm , 1,070 μm	4–8 cm	In progress
Sandia (2018)	Slot	Steel	700 kPa	1 μm	28.9 $\mu\text{m} \times 8.86$ mm	12.7 mm	In progress

*dp: particle diameter; D: diameter (for capillary); H \times W: height \times width (for slot or crack); L: length

2. OVERVIEW

This section presents an overview of publicly available data on stress corrosion cracking characteristics including shape, roughness, opening displacement and estimated leakage rate. The currently available data are used as a starting point for the development of gas flow and aerosol leakage models. Additional details and compilation of available data in the open literature on canister characteristics, e.g., pressure, temperature, heat load, environmental conditions, etc., and past models and experiments involving aerosol transport can be found in [Chatzidakis 2018a].

2.1 Stress Corrosion Cracking Characteristics

Stress corrosion cracking (SCC) is a localized process of degradation that can initiate cracks by the combined actions of stress (residual or applied) and corrosion (electrochemical). Three conditions are necessary for SCC to occur: tensile stress, aggressive electrolyte, and susceptible material. The most likely starting points where cracks can develop are the zones affected by weld heat or crevices in the canister surface. The tendency for cracking depends on temperature, relative humidity, time of exposure, and chemistry. After a few decades of storage, canister surface temperatures are in the regime for corrosion-induced degradation (Figure 1). However, cracking can occur at higher temperatures if conditions allow deliquescence of corrosion agents.

Most intergranular-SCC develop next to welds with straight or winding cracks oriented almost parallel to the weld. Single cracking is most common but occasionally two cracks are formed on each side of the weld. In the through thickness direction intergranular-SCC is typically winding or lightly bend and macroscopic branching is rare. The surface roughness is normally on a grain size magnitude and the cracks are particularly narrow providing secondary corrosion is small.

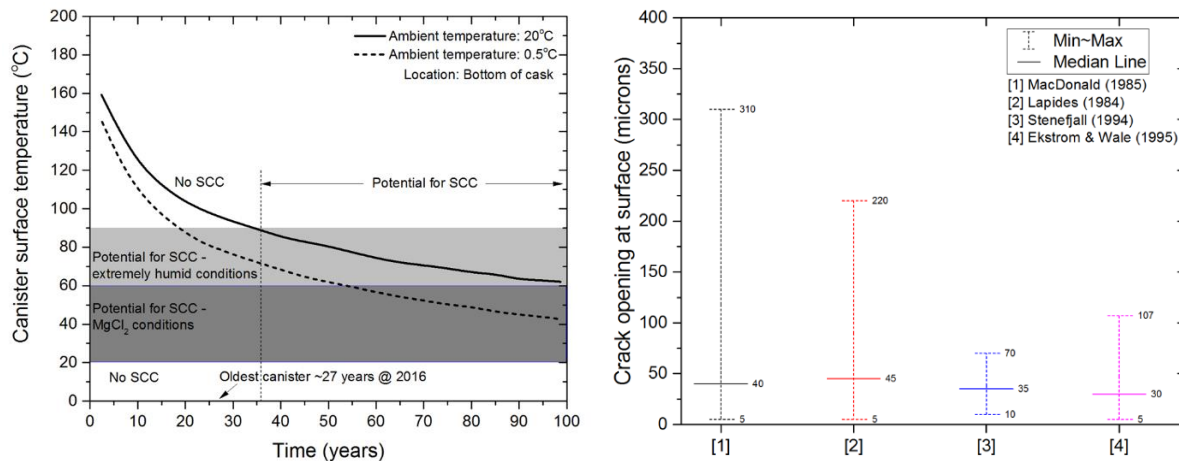


Figure 1. Left: Estimated surface temperatures over total storage time and illustration of potential SCC regime. Right: Crack opening displacement median, minimum and maximum values.

2.1.1 Crack opening and width

Experiments have shown that SCC exhibits crack opening displacements of 15–30 μm (Figure 1). Crack width midway between the surface and the crack tip is smaller. Crack width at tip is on the order of 1 μm . Table 3 shows statistics from 65 cracks for crack width at surface, midway and at tip. It is observed that the crack width decreases away from the surface.

Table 3. Crack width at surface, midway and at tip of IGSCC in austenitic stainless steels [SKI 2006].

	Crack width at surface (µm)	Crack width at midway (µm)	Crack width at tip (µm)
Min	3	2	1
Max	160	133	25
Mean	37.7	22.5	4.7
Median	30	16	3
Std. dev.	28.7	22.0	4.74

2.1.2 Orientation

Due to maximum sensitization the cracks typically are oriented parallel to welds and located in the heat affected zone. The crack is expected to form in the region of most severe sensitization. Thus, the distance between the crack and the weld fusion line is dependent on the welding parameters, number of weld beads, wall thickness etc. Furthermore, the heat input is a crucial parameter. The typical distance found in this work is between 0 and 10 mm. For single run welding the distance may be calculated. However, for multi-run welding the situation is more complicated, and maximum sensitization may occur very close to the root run fusion line, because the second weld run may sensitize the root run HAZ.

2.1.3 Shape

Typical shape in surface direction is straight or winding. Most cases showed a continuous crack running approximately at a constant distance from the weld. However, there are exceptions showing discontinuous cracking and cracks growing at various distances from weld.

2.1.4 Location

Recently, a welded, Type 304L stainless steel coupon test as part of a qualification program for plutonium storage containers developed stress corrosion cracks when exposed, at room temperature, to salt mixtures that contained only about 0.6 wt% moisture. The stress corrosion cracks initiated in the heat affected region of the weld and propagated along the HAZ and into the base metal. Such observations are clearly relevant to the welded canisters placed in dry storage. The number of cracks is typically one but exceptionally up to six separate cracks have been observed. The orientation in the thickness direction is typically 90° but cracks commonly tend to bend towards the weld metal. Typical shape in the through thickness direction is winding due to the inter-granular growth. Curved cracks are common and crack growth tends to turn towards the weld. Crack growth into the weld metal is very unusual.

2.1.5 Roughness

The crack surface roughness has been evaluated from crack profiles derived from micrographs. It was found that the surface roughness is strongly influenced by the grain size. Table 4 shows surface roughness and grain size statistics derived from 69 crack measurements. Surface roughness is on the order of grain size. It can be seen that surface roughness varies from 8 to 200 µm with a median value of 68 µm. The grain size varies from 15 to 250 µm with a median value of 50 µm.

Table 4. Crack surface roughness and grain size of IGSCC in austenitic stainless steels [SKI 2006].

	Surface roughness (μm)	Grain size (μm)
Min	8	15
Max	200	250
Mean	70.7	69.6
Median	68	50
Std. dev.	39.6	51.9

2.1.6 Crack opening area and estimated leakage rate

Typical values for crack opening area vary from 0.004 to 0.025 cm² based on crack length 2.5 cm. Estimated leakage rates and exchange times to replace the helium in a canister with air for a variety of cases where parameters including the canister internal free volume and CISC crack opening area are shown in Table 5. The estimates assume a single through-wall crack. Pressurization is calculated to dissipate within one day for all canister designs when assuming a crack opening area of 0.025 cm². Cases with a crack opening area of 0.004 cm² required longer, up to 52 days. The values shown are maximum leak rate values, the leakage rate decays with time as the pressurization decreases.

Table 5. Estimated leakage rate and time to depressurization for some DPCs [EPRI 2017].

Cask model	Canister volume (cm ³)	Initial pressure (MPa)	Crack opening area (cm ²)	Leakage rate (cm ³ /s)	Time to depressurization (days)
HI-STORM 24	6.76E6	0.69	0.025	943	1
NUHOMS 32PT	3.77E6	0.10	0.025	484	1
UMS 24	5.74E6	0.10	0.025	431	1
MAGNASTOR 37	6.56E6	0.76	0.025	960	52
HI-STORM 24	6.76E6	0.69	0.004	28.7	52
NUHOMS 32PT	3.77E6	0.10	0.004	4.44	52

3. Aerosol Transport and Plugging Model

This section presents an overview of the phenomenological aerosol transport and plugging model. The model is described in more detail in [Chatzidakis 2018b and Chatzidakis 2019] and only the main features are summarized in this section. Overall, the model can predict important quantities such as plug mass, gas passed, plugging time, plug profile, and aerosol penetration or retained fraction.

3.1.1 Aerosol Transport Equation

The behavior of an aerosol within a volume may change due to processes that occur within it, processes referred to as internal, and due to processes that transport particles across the volume boundaries, referred to as external. Internal processes include coagulation, agglomeration, fragmentation and gas-to-particle conversions. External processes include transport across the boundaries due to gas flow, diffusion, particle motion as a results of temperature gradients, concentration gradients, gravitational settling and other external forces. All processes are described by a balance equation that is known as the general dynamic equation (GDE).

The GDE for the case of aerosol penetration through a microchannel assuming only external processes is reduced to a transport equation, which can be written as follows in one-dimensional form [Mitrakos et al. 2008; Chatzidakis and Scaglione 2019]:

$$\frac{dC(x,t)}{dt} + \frac{1}{A(x,t)} \frac{d}{dx} [A(x,t) \cdot u(x,t) \cdot C(x,t)] = -V_d(x,t) \frac{\chi(x,t)}{A(x,t)} C(x,t), \quad (1)$$

where C is the aerosol mass concentration, V_d is the deposition velocity, A is the cross-sectional area, χ is the wetted perimeter of the cross section and u is the gas velocity. All previous parameters are functions of the axial coordinate x and time t . The deposition velocity is calculated as the sum of the deposition velocities corresponding to each individual deposition mechanism, e.g., gravitational, diffusion, etc.

3.1.2 Flowrate

The aerosol transport equation given above can be applied to any cross-sectional shape for which the hydraulic diameter and mass flow rate are known. The mass flow rate Q_m can be written as a function of the pressure drop along the flow direction (Williams 1994):

$$p_u^2 - p_d^2 = R_g T Q_m^2 \int_0^L C_f(\text{Re}) \frac{\chi(x)}{A^3(x)} dx, \quad (2)$$

where x is the axial distance from the inlet of the crack (or capillary), p_u and p_d are the pressure at the upstream and at the downstream of the crack, respectively, L is the length of the duct, χ is the perimeter of the duct, and A is the cross sectional area. This equation can be solved numerically to determine the mass flow rate Q_m . When this is known, the velocity and volume flow rate can be calculated using mass continuity.

3.1.3 Deposition Mechanisms

Deposition mechanisms transport aerosol to the walls of a leak path due to gas flow, gradients or external forces. Four deposition mechanics are considered herein: gravitational settling, Brownian diffusion, inertial impaction, and eddy impaction for the case of turbulent flow conditions. These deposition mechanisms play a crucial role in aerosol retention within a microchannel and are described in more detail in a previous report [Chatzidakis 2018b]. Other deposition mechanisms such as electrophoresis, and diffusiophoresis are neglected, as rough calculations indicate that these mechanisms are relatively unimportant in the removal of particles in leak paths for conditions relevant to stress corrosion cracks.

3.1.4 Plugging

A leak path through which aerosol passes and deposited may become partially or completely plugged. The particulate matter will deposit on the surface, changing the internal geometry of the flow area. Eventually the plug mass will increase and will lead to a complete obstruction of the pathway.

The mass of the deposit up to any position S can be obtained in terms of the deposition velocity and the particle concentration, as follows:

$$M_{dep} = \int_0^S \int_0^t 2\pi R C V_d dx dt. \quad (3)$$

Assuming that the deposit material is homogeneous with a density equal to the density of the particles, then the volume of the deposit can be directly derived from its mass:

$$V_{dep} = \frac{M_{dep}}{\rho_p}. \quad (4)$$

In Eq. (4) above, density ρ_p is assumed to be the bulk material density. This approximation is more accurate for large particles that are deposited mainly by gravity or eddy impaction. The deposition of particles is assumed to occur uniformly on the path's circumference. This assumption is valid for mechanisms such as Brownian or turbulent diffusion or for eddy impaction, but it is approximate for directional mechanisms such as gravitational settling. Under this assumption, the change in radius due to plugging is related to the deposit volume, as follows:

$$dR = \frac{1}{2\pi R} \frac{dV_{dep}}{dx}. \quad (5)$$

The aerosol transport equation, Eq. (1), is solved using an implicit finite difference scheme. The upwind scheme is used for the discretization of the convection term, which is the second term on the left-hand side of Eq. (1). The duct radius is then updated according to Eq. (2) through calculating the amount of the deposited mass, as shown in Eqs. (3) and (4). All the numerical integrations required in this calculation are performed using the trapezoidal rule. The new cross section is then used for the aerosol calculations in the next step (Figure 2).

3.1.5 Depressurization and Transient State

The model described above assumes deposition only within a microchannel under constant (steady state) conditions, and it does not take any depressurization events into account that may influence deposition. To address these shortcomings, a depressurization equation was added to the model to account for pressure change over time (transient state). Furthermore, the model was extended to account for coagulation and deposition within a vessel such as canister, with dimensions much larger than that of a microchannel. In this case, aerosol reduction due to coagulation and deposition mechanisms within a large vessel and within a microchannel can be predicted before, during, and after depressurization.

Combining mass and energy conservation equations for vessel depressurization, one can arrive at the following formula:

$$\frac{dP_{vessel}}{dt} = - \frac{Q_m P_{vessel} \gamma_g}{M_{vessel}}, \quad (6)$$

where γ_g is the ratio of specific heat capacity at constant pressure and volume. Applying the forward Euler method (explicit) to iterate pressure over time, it is possible to follow the pressure changes in the system and extract the time when pressures will equalize.

3.1.6 Aerosol Coagulation and Deposition within Canister

The principle of mass conservation when applied to aerosol particles inside a canister is:

$$\frac{dC_1}{dt} = -K_{1c}C_1^2 - \frac{Q(t)C_1}{V_1} - (K_{1g} + K_{1d})C_1, \quad (7)$$

Where K_{1c} is the coagulation decay rate, C_1 is the particle concentration, t is time, Q is the volumetric flowrate, V_1 is the canister's free volume, K_{1g} is the particle decay rate due to gravitational settling, and K_{1d} is the particle decay rate due to diffusion to the surfaces. The first and second terms on the right side represents the rate at which particles are removed from the canister by coagulation and airflow. The third term represents the rate at which particles are removed by deposition mechanisms on surfaces other than a microchannel.

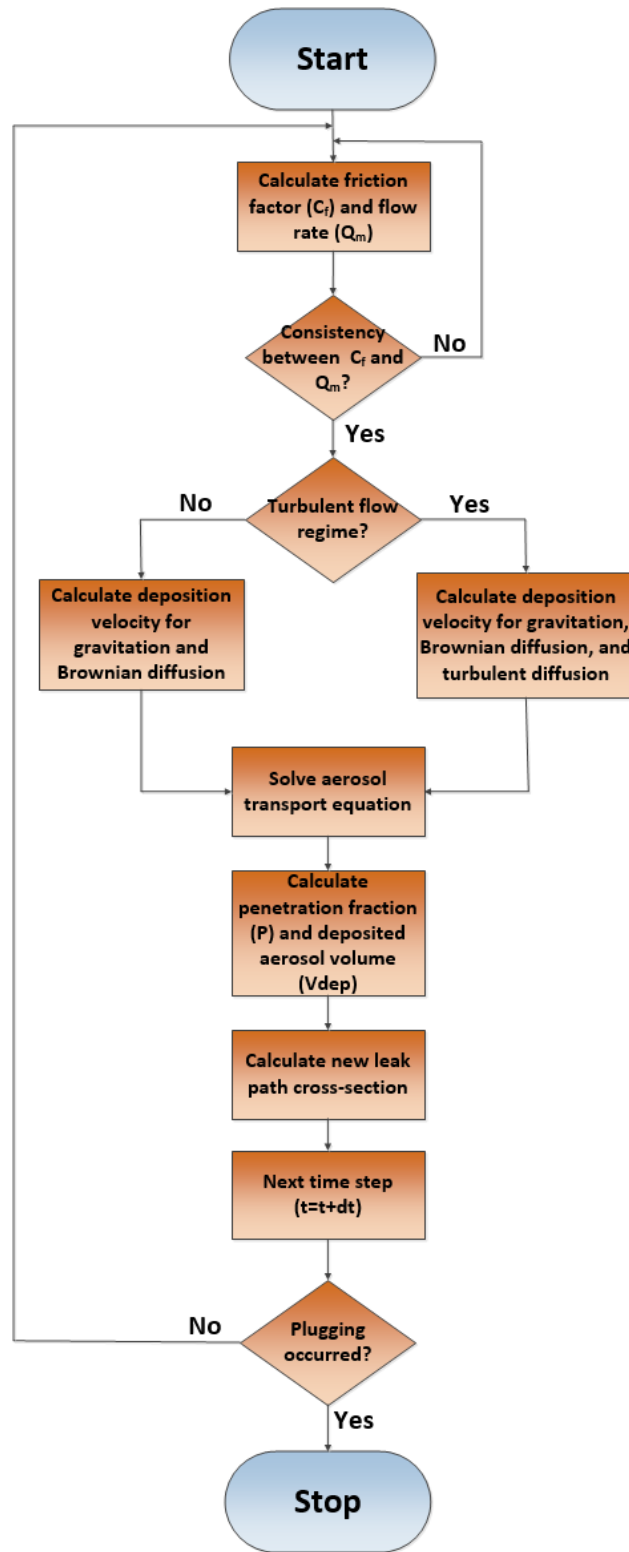


Figure 2. Block diagram for numerical solution of the aerosol transport equation [Chatzidakis 2018b].

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4. VALIDATION RESULTS

To evaluate the proposed aerosol transport and plugging model, the model described in Section 3 was benchmarked against real experimental cases of particle penetration and plugging in leak paths under a variety of conditions in tubes, slots, or real cracks. Four distinctive, independent types of experiments are presented. The first is based on recent Sandia measurements on microchannels [Sandia 2018]. The second and third experiments are focused on penetration of particles through the cracks of a naturally broken brick [Liu and Nazaroff 2003] and on penetration of particles through a cracked reinforced concrete sample [Gelain and Vendel 2007]. The fourth experiment focuses on penetration of particles through microcapillaries [Tian et al., 2017]. The validation results are described in more detail in [Chatzidakis 2019] and only the main results are summarized in this section.

4.1 Comparison with Sandia Experiments (2018)

The results of the present model vs. Sandia’s experimental measurements are shown in Figure 3. It is noted that the measurements were taken before aerosol was released into the tank, so there was no aerosol influence (pre-aerosol measurements). Good agreement is observed with experimental measurements.

The following observations are made:

- A flow rate based on laminar friction factor significantly overestimates the flow rate. It can be stated that the flow is not laminar, despite Reynolds number being less than 2,300.
- The friction factor correlation of Gelain (Gelain, 2007) that captures the laminar to transition region at $Re=5-10$ and was developed based on experimental data from concrete cracks underestimates the flow rate.
- Trials with different friction factor correlations were performed but none successfully reproduced the experimental measurements.
- A new friction factor correlation is needed to capture the measured flow rate.

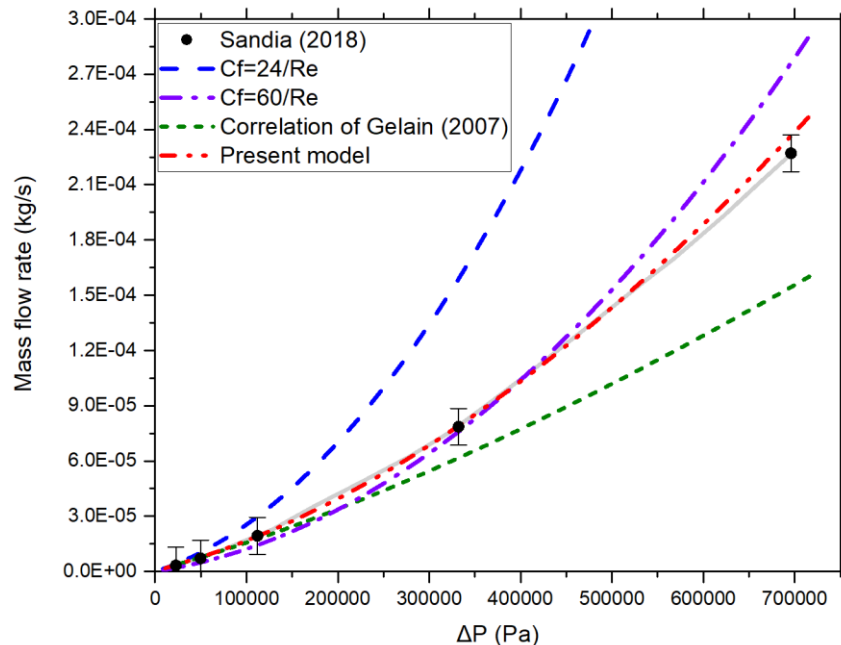


Figure 3. Flow rate vs. pressure differential (pre-aerosol measurements).

The depressurization equation, Eq. 6, was used to predict the mass flow rate over time. For tank volume 0.908 m^3 , the results are shown in Figure 4. Given the simplicity of the depressurization equation, the results are in good agreement with the experimental measurements although the difference appears to be larger as time progresses. This can be partially attributed to the simplifying assumptions that were made during the derivation of the depressurization equation. Further, the present aerosol model was in good agreement with the experimental measurements and predicted correctly the aerosol concentration within the source container (upstream) due to coagulation as shown in Figure 5. A coagulation constant of $2 \times 10^{-7} \text{ cm}^3/\text{s}$ was used.

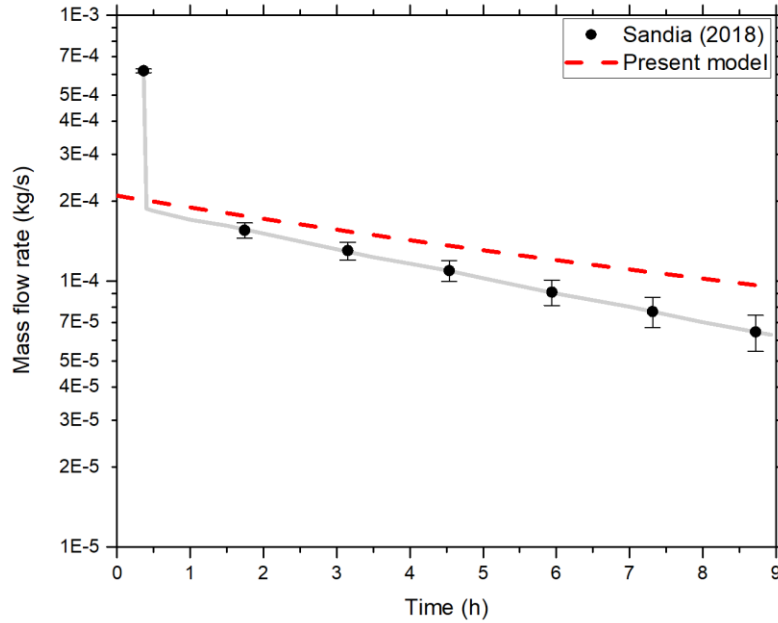


Figure 4. Flow rate vs. time during depressurization.

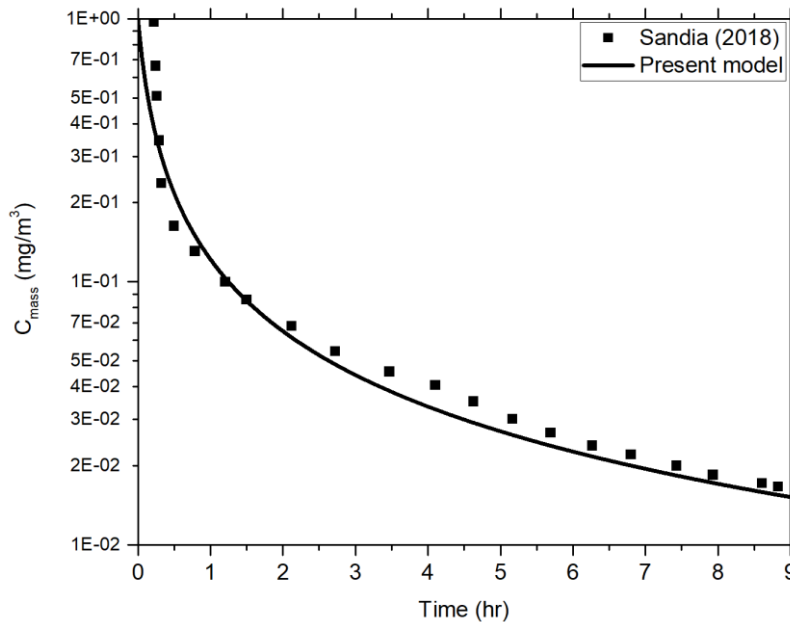


Figure 5. Upstream aerosol mass concentration as a function of time.

4.2 Comparison with Liu and Nazaroff (2003)

Liu and Nazaroff (2003) experimentally studied the penetration of particles through cracks of usual building materials. They used cracks of well-defined, controlled geometry by machining the materials samples, but they also created real cracks by breaking a brick. Results from the latter tests were selected in the present work to imitate a realistic case. The test conditions refer to a nominal leak path length of 4.5 cm, crack heights of 0.25 and 1 mm, and a pressure difference of 4 Pa. The authors measured the particle penetration fraction for particle sizes 0.02–7 μm . Figure 6 shows the penetration fraction of particles for two different crack heights as calculated with our numerical model and compares the calculated results with the measured data. The flow was laminar, so only two deposition mechanisms are accounted for in the calculations in this work: namely Brownian diffusion and gravitational settling. The calculated results from the global model of Gelain (2007) are also shown. The following observations are made:

- Generally, both models display similar performances, but the penetration fraction as calculated with Gelain's model (2007) underpredicts when crack height is 1 mm and overpredicts when crack height is 0.25 mm.
- The model of Gelain (2007) goes abruptly to zero for large particles in the 0.25 mm case. The model developed for the current effort predicts that the penetration fraction will asymptotically reach zero, a behavior more consistent with the measured data.

Overall, it is observed that particles with $d_p < 0.01 \mu\text{m}$ or $d_p > 4 \mu\text{m}$ will not penetrate a crack with a height less than 250 μm . These results agree with the results from Gelain and Vendel (2007).

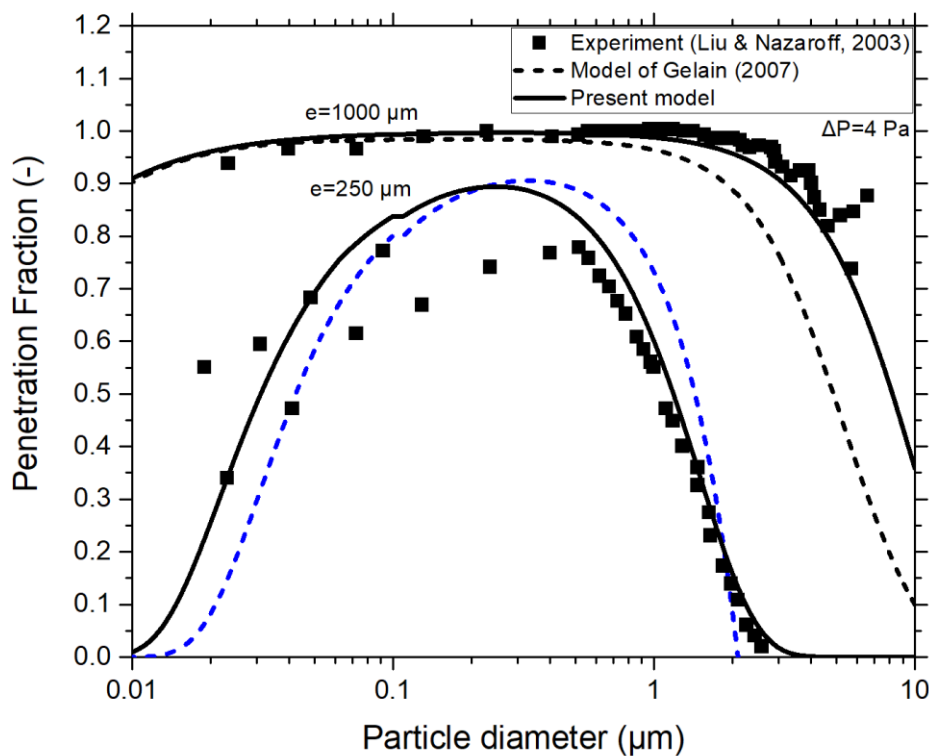


Figure 6. Penetration fraction of particles as a function of particle diameter.

4.3 Comparison with Gelain and Vendel (2007)

The experiments performed by Gelain and Vendel (2007) concern the penetration of particles through a real crack network that was created in a reinforced concrete slab measuring $128 \text{ cm} \times 75 \text{ cm} \times 10 \text{ cm}$. The sample wall was cracked by subjecting it to shear stresses from alternate directions. The tests were performed with monodisperse aerosols with particles between 50 nm and $4 \text{ }\mu\text{m}$. The aerosol penetration fraction was measured as a function of the imposed pressure difference across the concrete slab as a function of the flowrate leaking through the crack network. With the coarse particles of $4 \text{ }\mu\text{m}$, the aerosol was completely trapped in the cracks. The results for the $1 \text{ }\mu\text{m}$ aerosol diameter have shown a partial retention. Figures 7 and 8 show the penetration fraction of particles as calculated with the model developed for this effort, and they compare the calculated results with the measured data.

The present model gives satisfactory results when compared with the experimental measurements of Gelain and Vendel, and it is also in close agreement with their model. Generally, both models display similar performances. The present model gives a more realistic prediction for low flow rates. The model of Gelain (2007) predicts values higher than 1.0. The model developed for the current effort predicts that the penetration fraction will asymptotically reach 1.0, a behavior which is more consistent with the measured data. Particles of several microns can hardly penetrate through cracks because of the highly efficient removal of such particles by interaction deposition or gravitational settling.

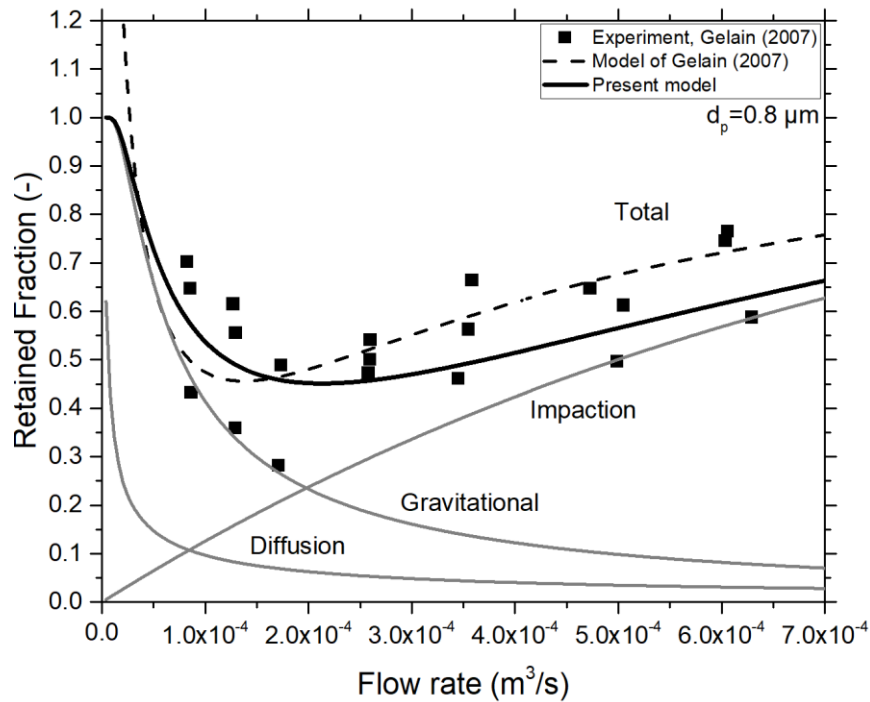


Figure 7. Deposition fractions for particles of aerodynamic diameter of $0.8 \text{ }\mu\text{m}$.

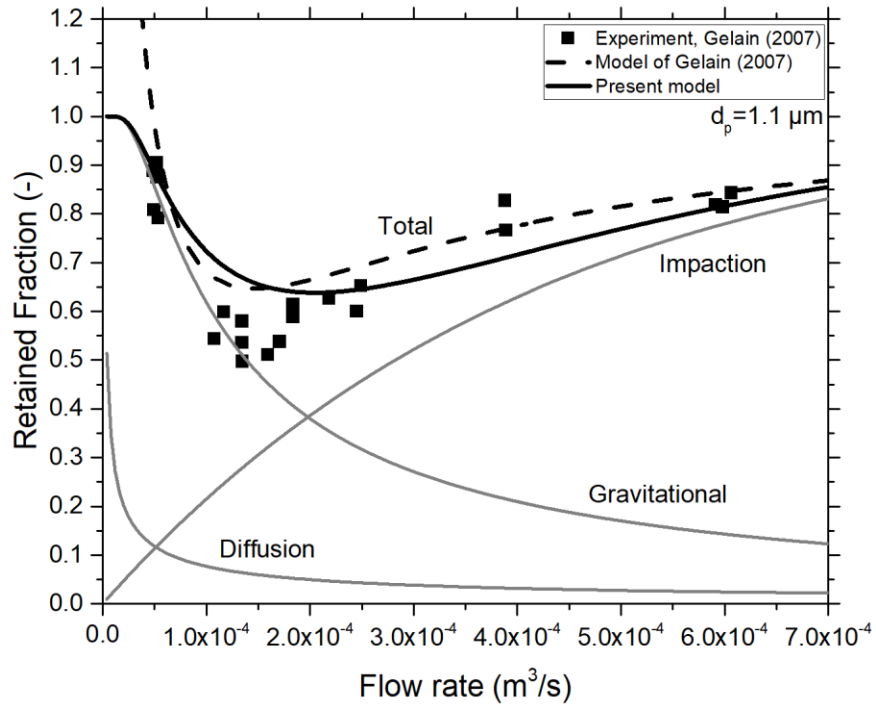


Figure 8. Deposition fractions for particles of aerodynamic diameter of 1.1 µm.

4.4 Comparison with Tian et al. (2017)

Tian et al. (2017) performed an experimental study of fine aerosol particles with size <0.3 µm through capillaries with bore sizes ranging from 5 to 20 µm and lengths from 10 mm to 80 mm. Pressure difference varies from 60 to 450 kPa. The results showed the aerosol penetration efficiency decreased significantly with increased capillary length but was identical for capillaries of same length but with different bore sizes. They also showed that the penetration efficiency correlates strongly with average flow velocity than with the air leakage rate.

The present aerosol model was in good agreement with the experimental measurements and predicted correctly the aerosol concentration within the source container due to coagulation as shown in Figure 9. A coagulation constant of $2 \times 10^{-9} \text{ cm}^3/\text{s}$ was used. Further, the model results capture the behavior of aerosol penetration efficiency for various bore sizes and flow velocities (Figure 10).

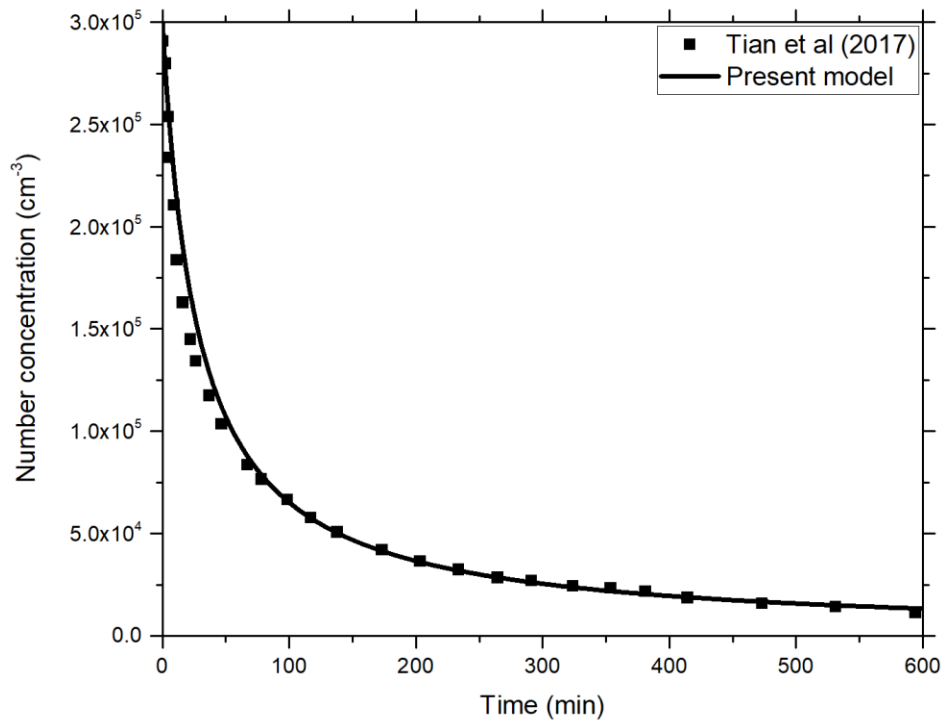


Figure 9. Aerosol concentration in container as a function of time. The aerosol reduction is due to coagulation.

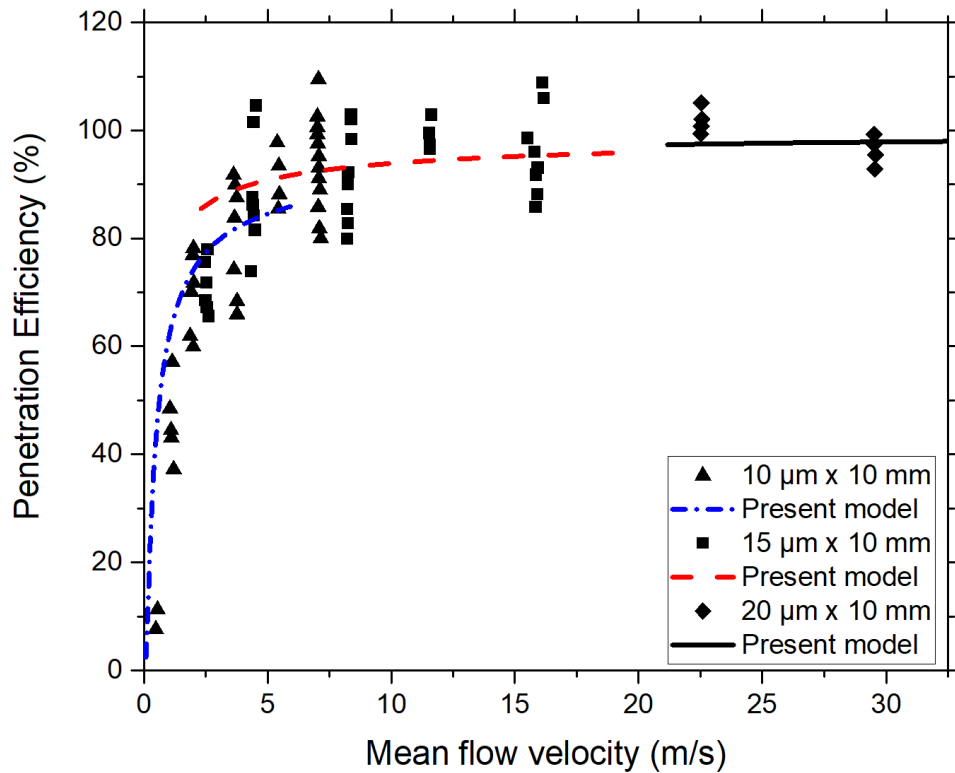


Figure 10. Aerosol penetration efficiency vs. average flow velocity in capillaries.

4.5 Flow rate benchmarking

To evaluate the flow rate prediction capabilities of the proposed model, two experiments were used: one in rectangular (crack-like) geometries [Gelain and Vendel 2007], and one in capillaries of various diameters [Sutter et al. 1979]. The results of the models vs. experimental measurements are shown in Figures 11 and 12. It is observed that the numerical model correctly predicts both the flowrates and Reynolds numbers for various pressure differences in laminar and transition flow regimes. For rectangular geometries, transition to turbulent flow regime starts at $Re=5-10$. For cylindrical geometries, transition to turbulent flow regime starts at $Re=400$. This is contrary to the widely used $Re=2300-4000$.

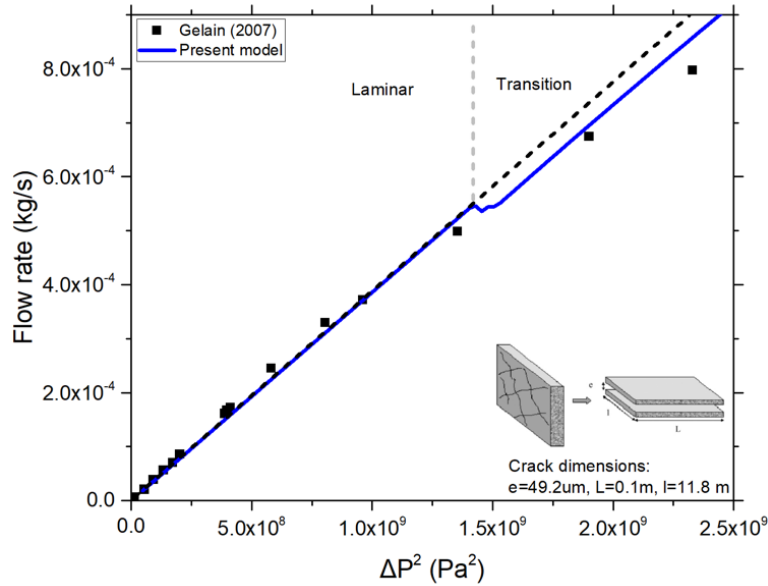


Figure 11. Flow rate vs. pressure difference for rectangular geometry [Gelain and Vendel, 2007].

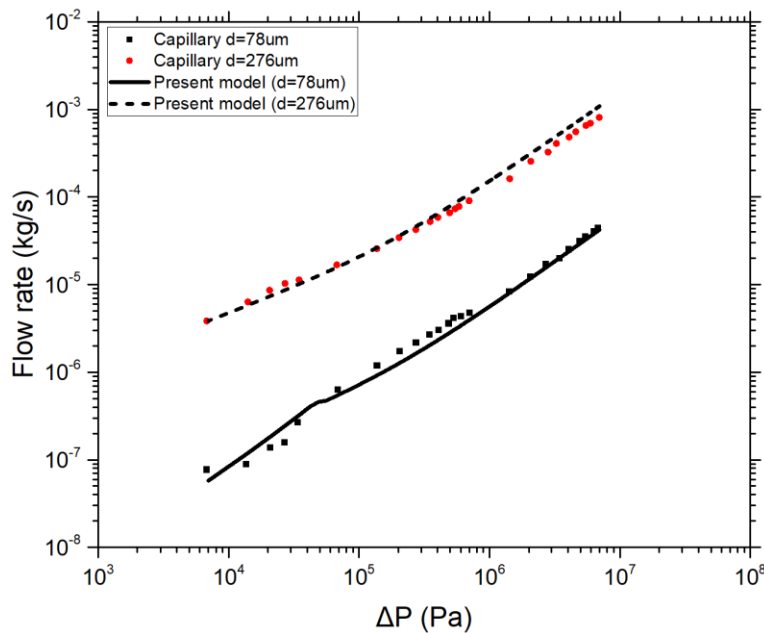


Figure 12. Flow rate vs. pressure difference for cylindrical geometry [Sutter et al., 1979].

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5. MODEL APPLICATION EXAMPLE

An example is discussed to demonstrate application of the developed phenomenological to estimate particle penetration through CISCC. In this example, particles are assumed to be spherical with a density of 8 g/cm^3 and with diameters ranging from 0.001 to $10 \text{ }\mu\text{m}$. The particle density was selected to represent particles with similar densities that may be released within a canister, such as UO_2 particles from fuel pellets. A uniform crack geometry is assumed throughout the channel, as well as a smooth inner surface and steady airflow through the crack. Three crack heights (crack opening) were selected: $e=30 \text{ }\mu\text{m}$, $e=50\mu\text{m}$, and $e=100 \text{ }\mu\text{m}$. Crack width was 10 mm , and crack length was 1.27 cm (0.5 in.). These dimensions are representative of real CISCC. In this case, the width of the crack in the third dimension is much larger than the crack opening so that airflow can be reasonably modeled as two dimensional without loss of generality. It is noted that in real cracks, irregular geometry and surface roughness might increase particle deposition significantly. This issue would be best explored by laboratory-scale experimental studies.

Figure 13 shows particle penetration fractions for a crack height of $30 \text{ }\mu\text{m}$ and three pressure differences: $\Delta P=50 \text{ Pa}$, 100 Pa , and 200 Pa . These higher-pressure differences were selected to better understand the required pressure that will allow significant particle penetration from such a small microcrack. The results suggest that particles having diameters in the range $0.1\text{--}0.5 \text{ }\mu\text{m}$ have the highest penetration across the whole particle spectrum. This is in agreement with earlier experimental results. Larger and smaller particles are readily removed in cracks under the gravitation settling and diffusion, respectively. The penetration factor becomes negligible for particles with diameters larger than $1 \text{ }\mu\text{m}$, even when a crack opening is $100 \text{ }\mu\text{m}$.

For a hypothetical crack height of $50 \text{ }\mu\text{m}$, particle penetration fraction is less than 30% . At a crack height of $100 \text{ }\mu\text{m}$, penetration is less than 90% . This translates to a reduction factor of 3, although crack height decreased by a factor of 2. For crack heights less than $30 \text{ }\mu\text{m}$, penetration is practically zero. This indicates that penetration varies strongly with crack height, and it significantly reduces with smaller crack heights.

Figure 13 shows that a significant pressure difference, larger than 50 Pa , is needed for considerable penetration to occur from a $30 \text{ }\mu\text{m}$ crack. Even when $\Delta P=200 \text{ Pa}$, penetration is less than 60% . For $\Delta P=50 \text{ Pa}$, penetration is less than 20% , and it is practically zero for smaller pressure difference. Figure 14 shows regimes for aerosol transport through CISCC as a function of pressure difference. Practically no aerosol release is predicted for cracks with opening displacements or heights less than $50 \text{ }\mu\text{m}$ when ambient conditions prevail.

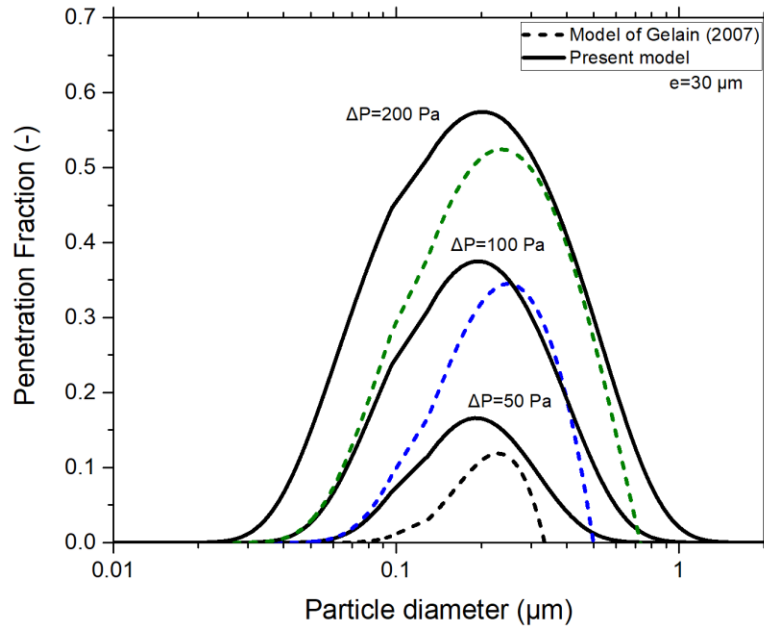


Figure 13. Penetration fraction as a function of particle diameter for crack heights $e=30 \mu\text{m}$ and $\Delta P=50 \text{ Pa}$, 100Pa , and 200 Pa .

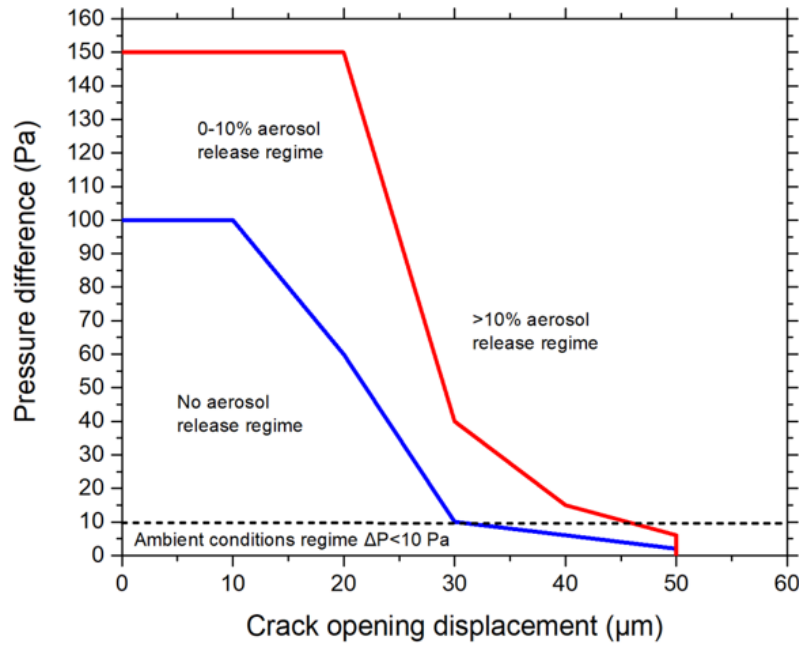


Figure 14. Regimes for aerosol transport through CISC as a function of pressure difference (penetration as a function of particle size spectrum is shown in upper right of figure). The term *ambient conditions* refers to conditions following canister depressurization. Highest penetration efficiency is observed for particles in the range of $0.1\text{--}0.5 \mu\text{m}$. No particles with diameters $>1 \mu\text{m}$ are expected to be released for cracks with opening displacement (height) less than $100 \mu\text{m}$.

6. SUMMARY

A phenomenological model is currently under development that enables the calculation of aerosol transport and retention in leak paths and that also accounts for plugging formation. The model assumes a one-dimensional flow through a hydraulically equivalent leak path. The description is dynamical, with changing duct geometry due to plugging, and it is also mechanistic. An extensive validation exercise (particle diameters: 0.01–10 μm and pressure difference up to 700 kPa) is in progress based on comparisons with experimental measurements and empirical correlations. The model predictions are in approximate agreement with experimental data and are reasonably representative.

Further progress will require (i) improvements to further refine the model and (ii) additional experimental studies for model validation. Experiments should include:

- Flow rates for various pressures to provide insight on flow regimes and develop friction factor correlations in a microchannel.
- Measurements of aerosol concentration in a canister, including polydisperse aerosol, to better understand aerosol reduction processes such as coagulation and deposition and for model validation.
- Tests that result in complete plugging of a microchannel to better understand aerosol plugging conditions and for model validation.

Advances in this area hold the promise of improving the accuracy of consequence assessments and reducing the uncertainty of radiological consequence predictive analyses by taking the filtering effect of leak path aerosol deposition and plugging into account in the source term.

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