Modeling analyses of radioactive aerosol flow and collection in mesoscopic impactor filters

Fenglei Niu a, Xiaochao Du a, Houbo Qi a,*, Mingqiang Yi b, Xu Yang a

a Beijing Key Laboratory of Passive Nuclear Power Safety and Technology, North China Electric Power University, Beijing 102206, China
b Microfluidic Foundry L.L.C., San Pablo, CA 94806, USA

Article info
Article history:
Received 3 June 2015
Received in revised form 28 December 2015
Accepted 29 December 2015
Available online xxx

Keywords:
Aerosol
Filter
Microfluid
MEMS inertial impactor

Abstract
The concentration of radioactive aerosols in the containment increases rapidly during the serious nuclear accidents. The common aerosol filters use mesh structures or filter papers, which can significantly increase the flow resistance due to the aerosol deposition and retard the containment pressure relief following the nuclear accidents. This paper proposes and studies a MEMS (Micro Electro Mechanical Systems) inertial impactor filters which can filter and collect 1 to 3 microns aerosol particles without filter papers. It can significantly reduce the flow resistance in filtering micron-size aerosol particles. The modeling method is given and the simulation results are analyzed.

© 2016 Elsevier Ltd. All rights reserved.

1. Introduction
When there is a rupture in the primary loop, the radioactive aerosols under the thermal dynamic action would be rapidly released into the internal environment, causing significant increase of radioactive aerosols concentration in the containment vessels (Fischer and Kanzleiter, 1999; Chen et al., 2011). It will cause serious damage to the atmospheric environment if such radioactive aerosols are directly emitted (Yi et al., 1999). Therefore, it is necessary to attenuate the radioactive aerosols before release. Attempts have been made by the FCVS designs to reduce the emission of the most penetrating sized particles by incorporating different retention techniques as well as by utilization of fine aerosol filters. The common filters collecting aerosols in nuclear power plants are FCVS with water scrubbers — droplet separators/deep bed fine aerosol filters, metal fiber filters with sorbent retention stage, sand bed filters (OECD, 2014), high efficiency air filters, and activated carbon filters (Allelein, 2009). Although these filters can collect and reduce a certain amount of radioactive dust, the filter papers they used can significantly increase the flow resistance in the course of aerosol deposition and therefore retard the containment pressure relief following the nuclear accidents, moreover, replacement of filter paper needs to be done regularly due to their mesh structure, and it has been a technical problem under the highly radioactive condition. In addition, the used filter papers become the new radioactive wastes (Arunkumar et al., 2007; Yu and Lin, 2011; Sun et al., 2012). The studies documented in this paper are concerned with a MEMS (Micro Electro Mechanical Systems) inertial impactor, which can collect micron sized particles with no need of changing the filter papers, and it can significantly reduce the flow resistance in filtering micron-size aerosol particles. MEMS belongs to the micro device technology, which has many potential benefits, such as high performance, low power consumption, good responsiveness, and low cost. MEMS devices would be easier to isolate, clean, and reuse. As for practical application, there is much lower possibility for the MEMS inertial impactor than the common filters to get overloaded or choked, because the diameter of the impactors’ flow channels is bigger than the porous media. The impactor’s collecting area can be designed to changeable parts depending on the needs of application.

In recent years, MEMS technology has made lots of progress. According to the survey, there is no precedent to collect plant aerosols based on MEMS technology. This study of MEMS device aims at filtering and collecting aerosols within 1–3 microns, which is a new attempt both on the design concept and technology.
2. Filter model development

When a particle laden air stream is caused to change direction suddenly, particles will tend to follow straight trajectories and to impact the opposite wall. It has been witnessed that the heavier (bigger) particles impact while the smaller particles follow the air stream. Using this theory, we design a novel filter to collect the aerosol releases from nuclear power plant containments. Unlike common filters, this impactor system does not have the electro part. It uses particle inertia to achieve separation and collection, which is a passively screening system. Based on the inertial effects in motion, the geometric model of MEMS inertial impactor for micron level aerosol collection was designed into a T tube with flat nozzle inlet, and the entrance width \( W \) is far less than its length. Therefore, a dimension in the direction of velocity can be neglected because of this design, the fluid flow can be simplified to a two-dimensional flow (As shown in Fig. 1), and the flow field is assumed to not be affected by the existence of the particles. We firstly computed the 2-D flow field around a T-junction, then the particles were seeded in the nozzle inlet and their trajectories were computed to determine whether they would impact or flow out. Our purpose is to find the optimized size that can achieve particle aerosol deposition based on the particle track.

Fig. 1 depicts the air streamlines and the particle trajectories in the inertial impactor. In our theoretical studies, the particles’ motion equations in a known flow field were analyzed. The relative importance of the various forces exerted on the particles was determined. An analytical criterion for determining whether the particle would impact or flow out was also developed. Based on the flow field computed with the commercial code FLUENT, the cut-off particle size was calculated as a function of the Reynolds number and the impaction distance.

3. Particle motion equations and asymptotic analysis

The particles’ motion is governed by Newton’s second law (Yi et al., 1999), mass times acceleration equals to the force exerted on them. In the carrier flow field, the particles will experience the Stokes drag force resulting from the relative velocity between the particle and the fluid. Assuming sphere particle of diameter \( d_p \), the Stokes drag force is 6\( \pi \nu V_r d_p \), in which \( V_r \) is the relative velocity between the particle and fluid. We also normalize the problem with length scale \( W \), velocity scale \( U \), and time scale \( \frac{W}{U} \). The non-dimensional particles’ motion equations are defined by Soo (1967) as below,

\[
\begin{align*}
Stk \frac{d^2x}{dt^2} &= U - \frac{dx}{dt} \\
Stk \frac{d^2y}{dt^2} &= V - \frac{dy}{dt}
\end{align*}
\]

where \((x, y)\) describe the instantaneous location of the particle at time \( t \), and \((u, v)\) are velocity of the flow field at point \((x, y)\). \(Stk\) (Stokes number) is the normalized particle size, which is defined by Soo (1967) as following equation,

\[
Stk = \frac{Re}{9} \left( \frac{\rho_p}{\rho_f} + \frac{1}{2} \right) \left( \frac{d_p}{W} \right)^2
\]

\[
Re = \frac{uW}{\gamma}
\]

In the above equation, \(\rho_p\) is the particle density, \(d_p\) is the particle diameter, \(u\) is the average inlet flow speed, \(W\) is the inlet nozzle width, and \(\gamma\) is the fluid kinematic viscosity. \(Stk\) is the ratio between the particles’ stopping distance in the quiescent fluid and the inlet nozzle’s width. The particles of large \(Stk\) will impact and can be collected while the particles of small \(Stk\) will flow out. Accounting for the fact that an air mass moves with the particle, the stokes number is based on the apparent density that includes, in addition to the particle’s mass, the virtual air mass of \(\left( \frac{1}{\gamma} \right) \rho_p\), where \(\rho_p\) is the particle mass.

In order to design the impactor that is used for the plant aerosols collection, we should find the relation among aerosol size, \(Re\), and the size of impactor. For each impactor design (\(D\)) and each flow field \(Re\), we will seed each size \((Stk)\) particle with the same speed as the fluid flow and then compute its trajectories inside the impactor to determine whether it will be collected or flow out. The fraction of collected particles is then calculated as the ratio of collected particles and total particles. By repeating the above calculations, we can obtain the fraction of collected particles \((E)\) as a function of the particle size \((Stk)\), which is defined as the efficiency curve of the inertial impactor.

Fig. 2 depicts the particle trajectories (dashed lines) and the flow streamlines (solid lines). It is clear that the particle trajectories deviate from the streamlines and the particles impact onto the bottom (impaction) plate. According to our simulations, no particles impacted when \(\sqrt{Stk} \leq 1.08\) and all particles impacted when \(\sqrt{Stk} \geq 1.09\).

After a mass of simulating calculations, we can get the efficiency curve as shown in Fig. 3, which reveals that the fraction of the collected particles \((E)\) is a function of the particles’ size for an “ideal” impactor with uniform inlet speed. That is, for the “ideal” impactor, particles that larger than a certain size (cut-off size) are collected at the impaction plate while smaller particles flow out of the impactor. The cut-off size \((\sqrt{Stk}_{50})\) is defined as the size \((\sqrt{Stk})\) at which 50% of the particles are collected. In order to quantify the “sharpness” of the efficiency curve, we define a sharpness factor \(Q_E\),

\[
Q_E = \int_{0}^{0.95} \sqrt{Stk} - \sqrt{Stk}_{50} \, dE
\]

In an ideal impactor, \(Q_E = 0\). The smaller the \(Q_E\), the sharper the efficiency curve. In the definition of \(Q_E\), the upper limit of the integral was chosen as 0.95 instead of 1 to make the data more reasonable. This is due to the difficulty of computing the particle trajectories near the wall since the velocity is nearly zero. Moreover, in experiments, it is hard to obtain data for collection efficiency close to 1.
4. A criterion for determining the impaction of particles

4.1. Particle’s requirements for the impaction

The performance of an impactor can be predicted by numerical methods, which solve the equations governing the fluid flow and particle motion (Yi et al., 1999). In many cases, it is only necessary to decide whether a particle could actually impact, given its position and velocity components at a point sufficiently close to the plate. In such cases, an analytical criterion can be developed for determining whether a particle impacts without following through the integration process until actual impact had occurred.

Our asymptotic solution for the flow field near the stagnation point suggests that the velocity decreases as a quadratic function of $y$. A linearly decreasing flow field velocity would require a nonphysical pressure singularity at the wall. Therefore, it’s necessary to develop different criteria to judge whether a particle impacts or not. We assume the particle has vertical velocity $v_0$ at $y = y_0$, and the fluid’s velocity is $v_f$ at $y = \Delta$.

1) Simplest (most conservative collision criterion):

Considering equation (3.1) and neglecting the quadratic term, we obtain that, for the particle to arrive at the wall, it needs,

$$-v_0 > \frac{2v_0}{\sqrt{Stk}} \quad (4.1)$$

2) Results based on Stokes flow near the wall:

We assume fluid velocity of the form $v = v_f \left(\frac{y}{\Delta}\right)^2$, the collision criterion is,
\[-v_0 > \frac{2y_0}{Stk} \quad 4 \frac{v_{11}y_0^3}{3Stk} \frac{v_0\Delta^2}{v_0^2} = \frac{2y_0}{Stk} \left( 1 - \frac{2v_{11}y_0^3}{3v_0\Delta^2} \right) \quad (4.2)\]

3) When pressure effects are considered, the equation is,
\[
Stk \frac{d^2y}{dt^2} = v_{1f} \left( \frac{y}{\Delta} - \frac{dy}{dt} - \frac{1}{9} \frac{d\rho}{W} \right)^2 \quad (4.3)
\]

Notice that additional work needs to be done to overcome the pressure gradient as the flow approaches the stagnation point. Therefore, a higher initial speed is needed for the particle to reach the wall. The impaction criterion is,
\[
-v_0 > \frac{2y_0}{Stk} \left( 1 - \frac{2v_{11}y_0^3}{3v_0\Delta^2} + \frac{2v_{11}}{9v_0\Delta^2} \left( \frac{d\rho}{W} \right)^2 \right) \quad (4.4)
\]

As we all know, the containment vessel pressure would increase rapidly when a serious accident takes place in nuclear power plants, and the aerosol particles would also have a large instantaneous speed, which is enough for the aerosol to crash into the MEMS inertial impactor. Therefore, all of the factors meet the requirements of being collected.

4.2. Calculations of particle’s trajectories and collection efficiency

The trajectories of particles and collection efficiency are calculated by the DPM model of the commercial code FLUENT, which is often used to calculate the discrete phase model. The velocity of particles is modeled uniformly with the same as flow speed, considering particles are affected by gravity, Brownian motion, drag force, thermophoresis force, Saffman force, pressure gradient force and buoyancy lift. If the particle was collected when it hit the floor, then the particle’s trajectories in MEMS inertial impactor can be traced by numerical simulation, and the collected percentage is obtained.

5. Affecting factors analysis for the impactor’s performance

In our study, the particles were assumed to be uniformly distributed at the nozzle inlet. In conditions consistent with a serious nuclear plant accident, aerosol density is regarded as fuel canning material which is 8030 times as dense as air. Next, we will discuss the specific relation between collection efficiency and Re, as well as the relation between collection efficiency and the geometrical size of MEMS inertial impactor filters.

5.1. The relation between Re and collection efficiency

For relatively high Reynolds numbers (Re > 500), Marple et al. (1974, 1987, 1991) and Marple and Liu (1975) computed performance curves for this type of an impactor. Here, we repeated similar calculations for the low Reynolds numbers (Re < 500) that are typical to mesoscopic impactor.

Fig. 4 shows the cut-off Stokes number, \((\sqrt{Stk})_{50}\) (the normalized critical cut-off particle diameter, \(d_p\) at 50\% recovery) as a function of the Reynolds number. As the Reynolds number increases, the cut-off particle size decreases. The reason for this phenomenon is that the larger fluid inertia would cause the streamlines to get closer to the impaction surface.

Fig. 5 schematically presents two streamlines originating at the same point at the entrance under different Reynolds numbers (Re1 > Re2). The smallest distance between the streamline and the impaction surface is denoted as (s), which is the distance that the particles need to cross in order for impact to occur. The larger the Reynolds number, the smaller the s. The dependence of s on the Reynolds number causes the dependence of the cut-off Stokes number on the Reynolds number. Furthermore, this dependence was stronger for smaller Reynolds numbers. That means the dependence of the cut-off Stokes number on the Reynolds number is stronger in mesoscopic impactor than in traditional ones.

5.2. The relation between filter geometrical size and collection efficiency

In our simulations, particles were treated as spheres with finite diameter \(d_p\), not a point. Since the dependence of the cut-off size on the Reynolds number decreases as the Reynolds number increases, it is desirable to operate the impactor at as high a Reynolds numbers as possible to minimize its sensitivity to fluctuations in the flow rate. Unfortunately, high Reynolds number operation is difficult to achieve in a mesoscopic impactor. By reducing the impaction distance, one can reduce the dependence of the cut-off
size on the Reynolds number. For example, when \( \frac{Y}{W} = \frac{1}{2} \), the dependence of the cut-off size on the Reynolds number is weaker than when \( \frac{Y}{W} = 1 \).

The effect of the impaction distance on the cut-off Stokes number is illustrated in Fig. 6. As the impact distance \( Y \) increases, the \( \sqrt{\text{Stk}} \) increases nearly linearly when \( \text{Re} = 10 \). As shown in Fig. 5, the distance required for the particle to impact (\( s \)) is proportional to the impaction distance when the pattern of the streamlines changes in proportion to the impaction distance. Since the Stokes number is the particle's stopping distance, this means that the cut-off particle size also changes in proportion to the impaction distance. This dependence would flatten out when \( s \) does not vary with the impaction distance any more. After the simulation calculation, we obtained the relation between geometrical size \( Y/W \) and collection efficiency as shown in Fig. 7.

Fig. 7a and b shows the efficiency curves when \( Y/W = 1 \) (G1) and \( Y/W = \frac{1}{2} \) (G2), respectively. \( \rho_p = 1000 \) and \( \text{Re} = 1, 5, 10, 20, 50, 80 \). It indicated that when \( Y/W = \frac{1}{2} \), the dependence of efficiency curve on inlet velocity profile and the Reynolds number was weaker than when \( Y/W = 1 \). In addition, the efficiency curves were sharper than that of \( Y/W = \frac{1}{2} \).

6. Design and validation of MEMS inertial impactor filter

6.1. Filter design and simulation model establishment

Based on the analysis above and the environmental condition of containment under a serious accident, we can design the filter size and have it meet filtering requirements. Though the aerosol is mixture which contained a huge range of materials and chemical compounds, the density of the fuel cladding material is much higher than any other compounds of aerosols, and makes up a large percent of the mixture, so fuel cladding material has the most influence in the aerosols. Therefore, the density of the fuel cladding material (alloy material particles) whose density is 8030 times of air was used for the computation purpose in our simulation. Moreover, we supposed the particle size is 2 \( \mu \text{m} \) (OECD, 2014), designed the temperature as 150 °C (Lin, 2008). In the numerical simulation, the inlet pressure of gas phase and particles was designed as 0.407 MPa (Lin, 2008), considering particles under the force of gravity, Brownian motion, drag force, thermophoresis force, Saffman force and pressure gradient force.

According to the analysis, the diameter of T tube would be small enough to meet the condition of small Reynolds number. In our simulation, the inlet diameter of T tube was designed as \( W = 1 \text{ mm} \), outlet diameter \( Y = 0.5 \text{ mm} \), and height \( T = 1 \text{ mm} \). In order to ensure the particle's collision distance, we designed a long bottom of the collection plate with 13 mm.

In this paper, we set up inertial impact model using the above dimensions. Navier–Stokes equation and Continuity equation was built and solved by using the commercial code FLUENT for the simulation of flow field in T impactor. In computing, we assumed that the fluid inlet velocity is 6 m/s according to the nuclear power plant accident conditions.
6.2. Verify the impactor size by numerical simulation

6.2.1. Establishment of the continuous flow field in the impactor

This study is to simulate the air flow field of micro scales impactor. According to the equations (3.2) and (3.3), using the data in 6.1, we have calculated the Re in this simulation as 340. In terms of the theory, the fluid can be regarded as incompressible fluid under this condition. With the application of the commercial code FLUENT, we have obtained the flow field as shown in Fig. 8.

Since the aerosol particles are small and easily affected by air flow field, rebound phenomenon may appear after particle's deposition, which reduces the collection efficiency. In engineering design, we often design collecting groove to improve collection efficiency. The flow field in ladder bottom collector and conical bottom collector are shown as Fig. 9.

6.2.2. The establishment of the discrete phase track calculation model

In the commercial code FLUENT, the discrete phase particle track can be solved by integrating the Laplace coordinates of particle reaction differential equation, the force equilibrium equation of particles under the Cartesian coordinates (x direction) is indicated as the equation below (Ru et al., 2013).

\[
\frac{dp}{dt} = F_D(u - u_p) + \frac{g_s(p_p - \rho)}{\rho_p} + F_x
\]  

(6.1)

where \(F_D(u - u_p)\) is particles' drag force of unit mass, N/kg; \(u\) is the velocity of fluid, m/s; \(u_p\) is particle velocity, m/s; \(\rho\) is fluid density, kg/m\(^3\); \(p_p\) is grain density, kg/m\(^3\).

In this paper, simulating the diameter of the aerosol particle releases from containment as 2 \(\mu\)m, which is suitable for Stokes drag force formula, \(F_D = \frac{18m\rho_u}{p_pC_C}\) where \(m\) is the dynamic viscosity of fluid, Pa s; coefficient \(C_C\) is the Cunningham correction of Stokes. Drag force formula (taking particle surface velocity slip of rarefied gas dynamics into account), \(\lambda\) is gas molecule mean free path, m.

6.2.3. Verification of the impactor by numerical simulation

Particles movement obeys Newton's second law in the simulation. In the flow field, particles would have relative velocity because of the Stokes drag between particles and fluid. We can use the particle track model to simulate gas phase and particle phase, and the coupling effect between the two phases. In order to calculate incoming particles, the boundary of particle phase is set to escape surface at the inlet and outlet. Walls are all set to the trap surface. The experiment simulated particles movement under the small Reynolds number. The condition of gas phase includes entrance speed and free exits. After grid sensitivity analysis, taking precision and efficiency into account, we used the model under the scenario of 39,414 grid nodes. According to the actual situation of nuclear power plant, the aerosol injected into containment vessel when accidents take place can be assumed as liquid alloy particles with relative density to air, \(\rho = 8030\). From the equation (3.2), we can get \(\text{Stk} = 1.21\) which means \(\sqrt{\text{Stk}} = 1.1 > 1.09\). According to the previous analysis, if the design is reasonable, the particles would be all collected. By using the DPM model of the code FLUENT, we can also obtain the particle trajectories and collection percentages.

7. Impactor fabrication

The MEMS technology was a mature processing technology that has been finding numerous applications in industry. MEMS technology was used in fabricating stand-alone, single stage impactors. Using layered manufacturing, the impactor was machined in green ceramic tapes (DuPont, LTCC 951, nominal thicknesses ~250 m and 100 m). The impactor was fully assembled and co-fired. Subsequent
to the machining, internal cavities were filled with a graphite-organic binder mixture to prevent process-induced deformations, the layers were stacked together, laminated, and cofired (Bau et al., 1998). During the firing process, the organic binder burnt out and alumina particles and the glass sintered to form a rigid, monolithic block with internal fluidic passages. Fig. 10 depicts a cross-section of an impactor made out of 7 layers (from top to bottom) of ceramic tapes. Layers 1–3 contain the nozzle; layers 4–6 house the impactor’s cavity and layer 7 houses the exit ports (Each layer is about 230 m thick after firing, and the nozzle size (the top slot) is about 5 mm*500 m). Fig. 11a and Fig. 11b respectively show photographs of the top and bottom views of an impactor. Fig. 11c is an image of a diced impactor’s cross-section. The slot shown in Fig. 11a is the entrance to the intake nozzle. The two slots on the bottom serve to exhaust the gas stream. The gas stream was drawn through the impactor by inducing a vacuum downstream of the device.

The real object of impactor was shown in Fig. 12, inside the rubber is a real T-end impactor, inlet on the side of the silicon surface while two exports on the border of silicon and rubber.

We note in passing that a few impactors can be connected in parallel to accommodate high flow rates. Furthermore, a number of impactors can be connected in series to form a multi-stage impactor that makes the aerosols inside the containment to be collected efficiently.

8. Conclusions

In the process of numerical simulation, setting temperature for 150 °C and pressure for 0.407 MPa based on the nuclear power plant accident situation. We supposed that the particles rush into T tube with uniform speed as the same value of flow field. Figs. 13 and 14 show the particle track and the percentage of particle collection, respectively.

Simulating the same process, particle tracks in two impactors with different collecting groove were obtained and shown as Fig. 15.
From results shown in Figs. 13–15, it indicates that all the aerosols were collected in the MEMS inertial impactor filter, which proves that the size of impactor is reasonable, and the theory we put forward is feasible. It also proves that using MEMS inertial impactor filter to collect aerosol in containment vessel is feasible. Besides, collecting groove can improve the collection efficiency. Since the collected speed of the particles was reduced by collecting groove (particle speed in figure orderly increased from color blue to red), the possibility of rebound was also reduced. It can be demonstrated in Fig. 15, ladder bottom collector has larger blue collected area than conical bottom collector, so it become a better choice for aerosol collection, the design of collecting groove has a certain value in practical engineering application.

(2) From the simulation results analysis, it demonstrated that particles in MEMS inertial impactor filter were attenuated quickly, so the length of the bottom plate is long enough for the good collection efficiency.

(3) MEMS inertial impactor filter has many advantages, such as miniaturization, low cost, high precision and good dynamic characteristics, which made it applicable for the special environment of nuclear power plant containment vessel. In practice, it can be arranged in series in containment vessel to increase the filtering efficiency. The concept that using MEMS inertial impactor filter to attenuate micron radioactive aerosols is feasible and has practical significance.

It would cause serious pollution if the radioactive aerosols of containment vessels were released into the air without filtering. How to collect and attenuate with a simple and effective method has always been a problem. Based on the analysis and demonstration in this paper, application of MEMS Inertial impactor filter to attenuate and filter aerosol in containment vessel under the accident cases of nuclear power plant is feasible. If this method is applied successfully, it will make up for the deficiencies of existing aerosol filtration method, and become an innovative method for aerosols attenuation which will prevent the radioactive aerosols from escaping effectively.

This paper does not discuss the influence of radioactivity on particle transport phenomena. Radioactive particles can heat up the surrounding gas which will change the gas properties and, in consequence, change the transport phenomena. In the further simulation we will consider its effects. Moreover, in order to get more reasonable results, in the future work when we calculate for the condition of the mixture aerosols, we will use the aerodynamic diameter to consider the effects of internal voids and agglomerates.

Acknowledgments

This research is supported by the National Natural Science Foundation of China (91326108) and the Reactor System Design Technology Laboratory (HT-A100K-02-2014007).
References


