Investigation of differences of phenomena of diffusiophoresis and thermophoresis from aerosol deposition in modified ART Mod 2 code

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Abstract. Fission product behavior assessment in containment vessel (CV) is one of the important areas in safety analyses because the CV is the final release protection. Modified ART Mod 2 code is used to study aerosol deposition phenomena in the CV. From Phébus FPT experiments, the phenomena of diffusiophoresis and thermophoresis on wet condensers were occurred in the CV. The two phenomena are recognized to be the same thing. However, this is not a universal view on these phenomena, which are evaluated separately in the modified ART Mod 2 code. In previous study on the modified ART Mod 2 calculation of Economic Simplified Boiling Water Reactor (ESBWR) and Phébus FPT experiments, there was more diffusiophoresis than thermophoresis in the case of simulating single volume of the CV while there was more thermophoresis for multiple volume case. This research aim is to conduct a ceteris paribus sensitivity analysis of representative parameters affecting diffusiophoresis and thermophoresis namely aerosol size, pressure, and gas temperature, under different nodalizations in the modified ART Mod 2 code using the Phébus FPT experiments to investigate the differences. As a result, differences of gas temperature between atmosphere and wall in single volume most affect diffusiophoresis while differences of temperature between atmosphere and wall of multiple volumes most affect thermophoresis.

1. Introduction

Thailand Institute of Nuclear Technology (TINT) has started studies related to assessments of postulated severe accident (SA) of nuclear power plants (NPPs) since 2012. The assessment is divided into three parts. The first part is an assessment of thermal hydraulic characteristics in the reactor cooling system (RCS) using RELAP5 code [1]. The second part is an assessment of atmospheric dispersion of the radionuclide from the NPPs into environment [2, 3]. The third part is an assessment of fission product behavior in containment vessel (CV) [4, 5] which helps link the first two parts in order to understand the whole sequence of the SA. This research focuses on the part of assessment of fission product behavior in the CV where ART Mod 2 is used.

ART Mod 2 code was developed by Japan Atomic Energy Agency (JAEA) and had been actively updated until 1997 [6]. Then ART Mod 2 was modified aerosol deposition models to study aerosol depositions of cesium compounds by TINT [5]. Generally, ART Mod 2 is used to study aerosol deposition in the CV which divided to main four phenomena namely gravitational settling, Brownian diffusion, diffusiophoresis and thermophoresis [6]. However, there are many other codes which also
study the four deposition phenomena of fission product as in ART Mod 2, such as MELCOR 2.1 of the United States Nuclear Regulatory Commission (U.S.NRC) [7], CONTAIN 2.0 of U.S.NRC [8], ASTEC 2.1 of Institut de radioprotection et de sûreté nucléaire (IRSN) [9] and COCOSYS 1.2 of Gesellschaft für Anlagen und Reaktorsicherheit (GRS) [10].

In the previous study of fission product behavior, the research was started from simulation of Economic Simplified Boiling Water Reactor (ESBWR) using ART Mod 2 code [4]. The simulation of multiple volume case of ESBWR showed a lot of depositions of thermophoresis on wall of the CV. Then, the study on aerosol deposition of cesium compounds was conducted in a single volume case for Phébus FPT experiments using ART Mod 2 code and modified ART Mod 2 code [5]. It is found that diffusiophoresis dominates deposition on wall of the CV [5]. Actually, thermophoresis and diffusiophoresis are perhaps considered the same phenomenon such as the Phébus FPT experiments [11]. Thermophoresis phenomenon depends on the gradient of temperature of system while diffusiophoresis depends on the gradient of pressure fraction and momentum transfer which is also attributed to the temperature difference [6]. However, from the two previous studies, there are differences of thermophoresis and diffusiophoresis under the different nodalizations. It is found that there was more diffusiophoresis than thermophoresis in the case of single volume but there was more thermophoresis in the case of multiple volumes.

Therefore, the objective of this research is to conduct a ceteris paribus sensitivity analysis (parameter survey) of representative parameters, namely aerosol size, pressure and temperature, affecting diffusiophoresis and thermophoresis on wet condensers in Phébus FPT3 experiment using modified ART Mod 2 code under single volume and multiple volumes nodalizations. Wet condensers are considered in this research because diffusiophoresis and thermophoresis were main phenomena on wet condensers of the Phébus FPT3 experiment [11].

The paper is divided into four sections. This section introduces the background and the objective of the study. The second section explains the Phébus FPT3 experiment. The third section contains results and discussions. The last section is the conclusions.

2. Phébus FPT3 experiment

Phébus FPT3 experiment of Institut de radioprotection et de sûreté nucléaire (IRSN) which was conducted to study consequences of reactor vessel when core meltdown accidents happened and observed fission product release into the environment [12]. The study on fission product behavior in the CV was included in Phébus FPT3 experiment.

Figure 1 shows the CV geometry of Phébus FPT3 [13]. The 10 m³ of the CV is divided into vertical wall, elliptic roof, elliptic bottom and sump wall. Inside of the CV of Phébus FPT3 includes condensers divided into dry and wet parts.

Design parameters and boundary conditions of the Phébus FPT3 experiment is shown in Table 1 [11, 13]. Aerosols are released from the steam generator through a small pipe into the lower part of the CV. The pipe is directed upward toward the condensers. The inlet steam to the bundle of the Phébus FPT3 experiment is under steam poor environment which means constantly fed at $5 \times 10^{-4}$ kg/s at 0-18,000 seconds.
### Table 1. Design parameters and boundary conditions of the Phébus FPT3 experiment.

| Design parameters          | Boundary conditions          |
|----------------------------|------------------------------|
| Diameter of containment [m]| Pressure [MPa]               |
| 1.8                        | 0.21                         |
| Height of containment [m]  | Wall temperature [K]         |
| 5                          | 383                          |
| Diameter of condenser [m]  | Wet condenser temperature [K]|
| 0.15                       | 363                          |
| Height of condenser [m]    | Dry condenser temperature [K]|
| 1.5                        | 393                          |
| Number of condensers       | Aerosol and gas temperature [K]|
| 3                          | 383                          |
| Diameter of sump [m]       | Sump temperature [K]         |
| 0.584                      | 363                          |
| Height of sump [m]         | Inlet steam flow rate [g/s]  |
| 0.5                        | 0.0005                       |

### 3. Results and Discussions

This section is divided to three subsections. The first subsection is the simulation conditions of single volume and multiple volumes in order to simulate condenser region of the Phébus FPT3 experiment using modified ART Mod 2. The second section is the results and discussions of ceteris paribus sensitivity analysis or parameter survey of the main parameters including aerosol size, pressure, and gas temperature. The third section is observation of ceteris paribus sensitivity analysis.

#### 3.1. Simulation conditions

In this study, the author focuses on phenomena of diffusiophoresis and thermophoresis of the Phébus FPT3 experiment. The two phenomena occur on wall of wet condensers in the CV [11]. Therefore, only wet condenser part is simulated using modified ART Mod 2 code under single volume and multiple volume nodalizations to understand the two phenomena. This simulation uses volume of wet condenser conserving height and area of the three condensers. For boundary conditions of wet condenser, pressure and gas temperature are 2.1 bar and 383 K respectively. Wall temperature of wet condenser is fixed at 363 K. Steam flow rate and the mass flow rate of cesium hydroxide (CsOH) aerosol at the condenser volume from RELAP5 Mod 3.3 [16] are used to calculate in modified ART Mod 2 code [17]. Figure 2 shows steam flow rate at wet condenser which was evaluated from inlet steam to the bundle of the Phébus FPT3 experiment [17]. It is found that there is dropped trend of steam flow rate in Figure 2 in ranges of 9,000 – 13,000 seconds because of effect of steam reaction with other substances in the Phébus FPT3 experiment. CsOH is selected for the simulation because there are most chance for generation of aerosol of cesium compound which can also represent other aerosol of cesium compounds such as cesium molybdate (Cs₂MoO₄) due to equilibrium reaction [17]. Figure 3 shows CsOH mass flow rate at wet condenser [17]. It is found that CsOH had started releasing since 10,000 seconds until 17,000 seconds. This represent fission product release from SA. Table 2 shows CsOH parameters used to determine the aerosol size distribution for the simulation at degradation phase in the Phébus FPT3 experiment, including Aerodynamic Mass Median Diameter (AMMD) and Geometric Standard Deviation (GSD) [17].
Table 2. Mean characteristics of the CsOH at degradation phase in the Phébus FPT3 experiment.

| AMMD [µm] | GSD |
|-----------|-----|
| 1.45      | 2.7 |

For the simulation of wet condenser part, source is fed from center of wet condenser volume for the single volume case, and from the source volume for the multiple volume case. Figure 4 and Figure 5 show single volume nodalization and multiple volume nodalization of wet condenser part respectively. Diameter of the wet condenser volume is 0.90 m and the height is 1.64 m [17]. Source volume for multiple volume nodalization is the bottom part of the CV of the Phébus FPT3 experiment. Diameter of the source volume is 1.77 m and the height is 0.8 m [17].

3.2. Ceteris paribus sensitivity analysis (parameter survey)
This section shows ceteris paribus sensitivity analysis (parameter survey) results of aerosol size, pressure, and gas temperature on diffusiopheresis and thermophoresis under single volume and multiple volumes nodalizations in order to study the effect of change of the representative parameters. Probable values for maximum, minimum and average for the representative parameters are varied in order to study the effect of the two phenomena.

3.2.1. Ceteris paribus sensitivity analysis of aerosol size. Value of AMMD in Table 2 is varied within the range of 1.45×10⁻¹ to 1.45×10¹ µm to investigate occurrences of diffusiopheresis and thermophoresis. This aerosol size range is selected from aerosol size which covers degradation phase of the Phébus FPT3 experiment [11]. Figure 6 and Figure 7 show CsOH depositions from diffusiopheresis and thermophoresis, respectively, under single volume nodalization. For multiple volume, Figure 8 and Figure 9 show CsOH depositions from diffusiopheresis and thermophoresis, respectively, multiple volume nodalization. It is found that diffusiopheresis mostly occurs in single volume while thermophoresis mostly occurs in multiple volume. Increase of aerosol size affects increase of diffusiopheresis and decrease of thermophoresis. Large aerosol size affects increase of momentum transfer which affects increases of diffusiopheresis on wet condenser wall from the theory referred to [6].

On other hand, smaller aerosol size or small aerosol diameter affects increase of Knudsen number (Kn) which affects increase of thermophoresis on colder wall, at which this effect cause by increasing in thermal conductivity in the system which is confirmed by Epstein's experiment which is experiment to study parameters in thermophoresis under Kn changes [19].

3.2.2. Ceteris paribus sensitivity analysis of pressure. Pressure in the CV is varied within the range of 1.9-2.3 bar to investigate occurrences of diffusiopheresis and thermophoresis. This pressure range is selected from pressure which covers degradation phase of the Phébus FPT3 experiment [11]. Figure 10
and Figure 11 show CsOH depositions of diffusiopheresis and thermophoresis from ceteris paribus sensitivity analysis of pressure under single volume condition respectively. For multiple volumes, Figure 12 and Figure 13 show CsOH depositions of diffusiopheresis and thermophoresis from ceteris paribus sensitivity analysis of pressure under multiple volume condition respectively. It is found that most diffusiopheresis occurs in single volume while most thermophoresis occurs in multiple volumes. Increase of pressure directly affects increase of diffusiopheresis from the theory referred to [6]. However, there is decrease of thermophoresis because increase of pressure resists the occurrence of thermophoresis deposition on wall which is confirmed by Maxwell’s experiment which is prototype of experiment to study parameters in thermophoresis [19].

3.2.3. Ceteris paribus sensitivity analysis of gas temperature. Gas temperature in the CV is varied within the range of 373-393 K to investigate occurrences of phenomena of diffusiopheresis and thermophoresis. This temperature range is selected from gas temperature which covers degradation phase of the Phébus FPT3 experiment [11]. Figure 14 and Figure 15 show CsOH depositions of diffusiopheresis and thermophoresis from ceteris paribus sensitivity analysis of gas temperature under single volume condition respectively. For multiple volume, Figure 16 and Figure 17 show CsOH depositions of diffusiopheresis and thermophoresis from ceteris paribus sensitivity analysis of gas temperature under multiple volume condition respectively. It is found that most diffusiophoresis occurs in single volume while most thermophoresis occurs in multiple volumes. Increase of gas temperature directly affects increase of temperature gradient which affects increase of thermophoresis on wall from the theory referred to [6]. On the other hand, increase of gas temperature affects decrease of diffusiophoresis, because increase of gas temperature reduces chance to occur condensation of vapor in diffusiopheresis on wet condenser wall which is colder wall [5, 6].
Figure 10. CsOH deposition of diffusiopheresis from ceteris paribus sensitivity analysis of pressure under single volume condition.

Figure 11. CsOH deposition of thermophoresis from ceteris paribus sensitivity analysis of pressure under single volume condition.

Figure 12. CsOH deposition of diffusiopheresis from ceteris paribus sensitivity analysis of pressure under multiple volume condition.

Figure 13. CsOH deposition of thermophoresis from ceteris paribus sensitivity analysis of pressure under multiple volume condition.

Figure 14. CsOH deposition of diffusiopheresis from ceteris paribus sensitivity analysis of gas temperature under single volume condition.

Figure 15. CsOH deposition of thermophoresis from ceteris paribus sensitivity analysis of gas temperature under single volume condition.

Figure 16. CsOH deposition of diffusiopheresis from ceteris paribus sensitivity analysis of gas temperature under multiple volume condition.

Figure 17. CsOH deposition of thermophoresis from ceteris paribus sensitivity analysis of gas temperature under multiple volume condition.
3.3. Observation of ceteris paribus sensitivity analysis

From the results of ceteris paribus sensitivity analysis of aerosol size, pressure, and gas temperature, there are differences of percentage change of diffusiophoresis and thermophoresis for each parameter. Percentage changes are calculated from average value of deposition change per old deposition of each results in subsections of 3.2.1-3.2.3. Table 3 shows average percentage changes of diffusiophoresis and thermophoresis with aerosol size, pressure, and gas temperature under nodalizations of single volume and multiple volumes respectively. As a result, it is found that gas temperature parameter most affects change of diffusiophoresis and thermophoresis. From Table 3, percentage change due to gas temperature parameter for diffusiophoresis is 0.5% and for thermophoresis is 66.97% under nodalization of single volume. In addition, percentage change due to gas temperature parameter for diffusiophoresis is 0.0% and for thermophoresis is 2.84% under nodalization of multiple volumes.

However, from the theory of aerosol deposition referred to [6], aerosol size ($r$) is main parameter which should more affect diffusiophoresis and thermophoresis. From Figure 6, Figure 7 and Figure 9, percentage changes of the depositions from aerosol size tend to increase due to non-linear change. Therefore, if range of aerosol size is more extended, percentage changes of the depositions from aerosol size will tend to increase. In addition, it is also found that occurrences of diffusiophoresis and thermophoresis in the single volume agree with experimental results of the Phébus FPT3 experiment [11]. However, there is no diffusiophoresis in multiple volumes. This is because ART Mod 2 needs flow between volumes which is calculate from other code such as RELAP5 [17] to calculate diffusiophoresis. It is found that flow between volumes is very low which cannot determine circular flow in multiple volumes as in the Phébus FPT3 experiment as in three-dimensional code [20] thus there is no diffusiophoresis. From this results, modified ART Mod 2 is appropriate for simulation of single volume more than multiple volume.

Table 3. Percentage changes of diffusiophoresis and thermophoresis,

| Parameter       | Single volume |     | Multiple volumes |     |
|-----------------|---------------|-----|------------------|-----|
|                 | Diffusiophoresis | Thermophoresis | Diffusiophoresis | Thermophoresis |
| Aerosol size    | 0.42          | 44.38 | 0.00            | 0.45 |
| Pressure        | 0.17          | 12.10 | 0.00            | 0.47 |
| Gas temperature | 0.50          | 66.97 | 0.00            | 2.82 |

4. Conclusions

Ceteris paribus sensitivity analysis is conducted in order to investigate the influence of aerosol size, pressure and gas temperature on diffusiophoresis and thermophoresis which determine the depositions on wet condenser wall of the Phébus FPT3 experiment under single volume and multiple volumes nodalizations.

- Most diffusiophoresis occurs in single volume while most thermophoresis occurs in multiple volume. Large aerosol size affects increase of diffusiophoresis due to increase of momentum transfer while small aerosol size affects increase of thermophoresis due to increase of thermal conductivity. Increase of pressure directly affects increase of diffusiophoresis but it resists occurrence of thermophoresis. Increase of gas temperature directly affects increase of temperature gradient which affects increase of thermophoresis on wall while there are decrease of diffusiophoresis due to less chance to occur condensation of vapor in diffusiophoresis.

- Gas temperature most affects percentage changes of diffusiophoresis and thermophoresis on wet condenser from observation of percentage changes of the depositions.

- Modified ART Mod 2 is appropriate for simulation of single volume more than multiple volume due to limitation of parameter of flow between volumes.
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