THERMAL FLUID COUPLED ANALYSIS OF HYDROTHERMAL DESTRUCTION REACTOR

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Abstract. Multi-regionally coupled analysis of thermal fluid flow and heat conduction of solid using OpenFOAM is carried out to clarify the behavior of hydrothermal oxidative destruction reactor of polychlorinated biphenyls (PCBs). Internal fluid of the reactor assumes a single-phase hot water without chemical reactions considering temperature dependence of thermophysical properties. Compressible Navier-Stokes equation with buoyancy force and energy equation with gravity term are alternately solved for the thermal fluid analysis. In order to consider conjugate heat transfer between the internal fluid and the reactor vessel, two-regionally coupled analysis of the fluid and vessel was executed by chtMultiRegionFoam solver in the OpenFOAM. To verify coupling effect, the multi-regionally coupled analyses results were compared with thermal fluid analysis of the internal fluid or heat conduction analysis of the vessel.

1 INTRODUCTION

Hydrothermal oxidative destruction reactor decomposes polychlorinated biphenyls (PCBs, $C_{12}H_{(10-n)}Cl_n$) into water (H_2O), carbon dioxide (CO_2) and sodium chloride (NaCl) by dechlorination with sodium carbonate (Na_2CO_3) and oxidative decomposition with liquid oxygen (O_2) under high temperature 370 °C and high pressure 26.5 MPa [1]. In these reactor vessels, wall thinning due to corrosion was observed on bottom inner wall. At present, the reactors have been safely maintained and operated by adding a bottom

partition to prevent chemical sinking and supplying hot water to the reactor vessel bottom to control the temperature. Thermal fluid analysis of the hydrothermal oxidative destruction reactors is necessary to clarify the corrosion mechanism.

A finite volume analysis (FVA) code OpenFOAM [2] is used to perform a coupled analysis of the internal fluid flow and heat conduction in the reactor vessel with multi-region considering the conjugate heat transfer on the solid-liquid interface. This paper describes verification of the multi-regionally coupled analysis by comparing with single region analysis, which is thermal fluid analysis of the internal fluid or heat conduction analysis of the vessel body.

2 METHOD OF THE ANALYSIS

2.1 Governing equations

In this study, since chemical reactions in hydrothermal oxidative decomposition of PCBs are not considered, the internal fluid in the vessel assumes a single hot water. To analyze steady state of thermal fluid behavior in the vessel, the continuous equation, the compressible Navier-Stokes equations with buoyancy force, and the energy equation per unit mass with gravity terms are as follows:

$$\nabla \cdot (\rho \boldsymbol{u}) = 0 \tag{1}$$

$$\nabla \cdot (\rho \boldsymbol{u} \otimes \boldsymbol{u}) = -\nabla p_{\mathrm{rgh}} + \nabla \cdot \left[\mu \left\{ \nabla \otimes \boldsymbol{u} + (\nabla \otimes \boldsymbol{u})^{\mathrm{T}} \right\} \right] - \nabla \left(\frac{2}{3} \mu \nabla \cdot \boldsymbol{u} \right) - \boldsymbol{g} \cdot \boldsymbol{x} \nabla \rho \tag{2}$$

$$\nabla \cdot (\rho h \boldsymbol{u}) + \nabla \cdot (\rho K \boldsymbol{u}) = \nabla \cdot \left(\frac{\lambda}{c_p} \nabla h \right) + \rho \boldsymbol{u} \cdot \boldsymbol{g} \tag{3}$$

where $\boldsymbol{u}, h, K = \frac{1}{2} \boldsymbol{u} \cdot \boldsymbol{u}, \mu, \lambda, c_p, \boldsymbol{g}, \boldsymbol{x}$ and $p_{\mathrm{rgh}} = p - \rho \boldsymbol{g} \cdot \boldsymbol{x}$ are velocity vector, specific enthalpy, kinetic energy per unit mass, viscosity coefficient, thermal conductivity, specific heat, gravity acceleration vector, position vector and the absolute pressure p minus the static pressure, respectively. Although the energy equation (3) does not include heat generation term, the heat of chemical reaction is considered by a boundary condition. The thermophysical properties λ, c_p, μ depend on temperature T. Also, the equation of state, which describes density ρ, only depends on the temperature because of high pressure 26.5 MPa in the vessel. The turbulence is considered using the standard k-ε model.

The heat conduction equation without heat generation term for the reactor vessel body is as follow:

$$\nabla \cdot \left(\frac{\lambda}{\rho c_p} \nabla h \right) = 0 \tag{4}$$

where the thermophysical properties of the vessel body λ, ρ, c_p are assumed to be constant without considering the temperature dependence.

2.2 Method of the coupled analysis using OpenFOAM

In the coupled analysis of heat transfer between the internal fluid and the vessel body (solid), the continuities of temperature T and heat flux $(-\lambda \nabla T)$ are satisfied on the solid-liquid interface as follows:

$$T_{\mathrm{solid}} = T_{\mathrm{fluid}} \tag{5}$$

$$\lambda_{\mathrm{solid}} \nabla T_{\mathrm{solid}} = \lambda_{\mathrm{fluid}} \nabla T_{\mathrm{fluid}} \tag{6}$$
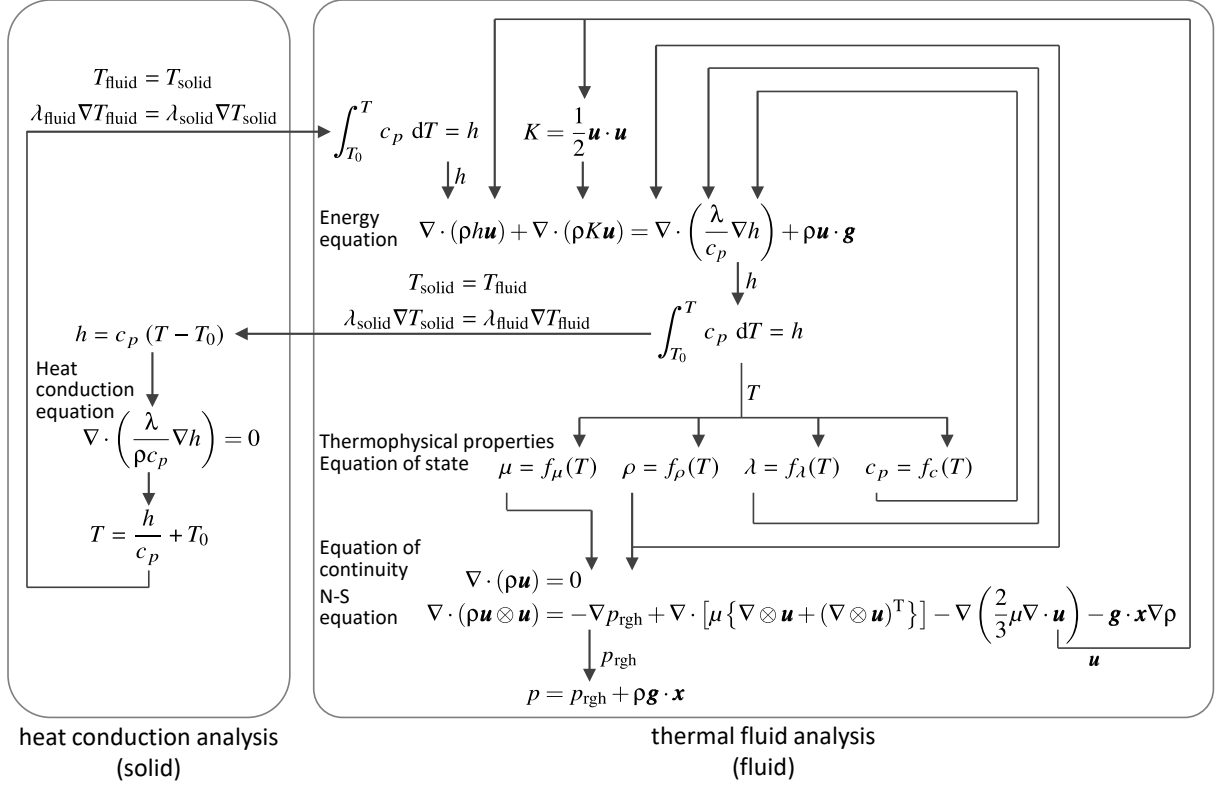
Figure 1: Flowchart of coupled analysis

Figure 1 shows flowchart of the coupled analysis. In the fluid region, the energy equation is solved to obtain specific enthalpy h and converted to temperature T. The thermophysical properties ρ, μ, λ, c_p are updated using temperature T, and fluid analysis is performed by solving compressible Navier-Stokes equation. In the solid region, the obtained temperature on the solid-liquid interface is used to analyze the heat conduction. The energy equation is updated using the solid-liquid interface temperature of the solid region and kinetic energy K. This calculation process is repeated until all solutions converge.

In this study, the standard solver chtMultiRegionFoam of OpenFOAM v7 [2] is used. In order to compare the analysis results, the thermal fluid analysis of the internal fluid using buoyantSimpleFoam and the unsteady heat transfer analysis of the vessel body using the laplacianFoam are also performed to compare the analysis results.

3 FINITE VOLUME MODEL AND ANALYSIS CONDITIONS

3.1 Construction of 3D finite volume model

In this study, 3-dimensional (3D) solid model shown in Fig. 2 was constructed using a 3D CAD software based on the configuration drawing of the actual reactor. Although there are various structure parts such as pressure sensing tubes inside the actual reactor, in this study, the analysis domain is from the bottom of the vessel to the height of 5 m in order to focus on the thermal flow phenomena at the bottom of the vessel.
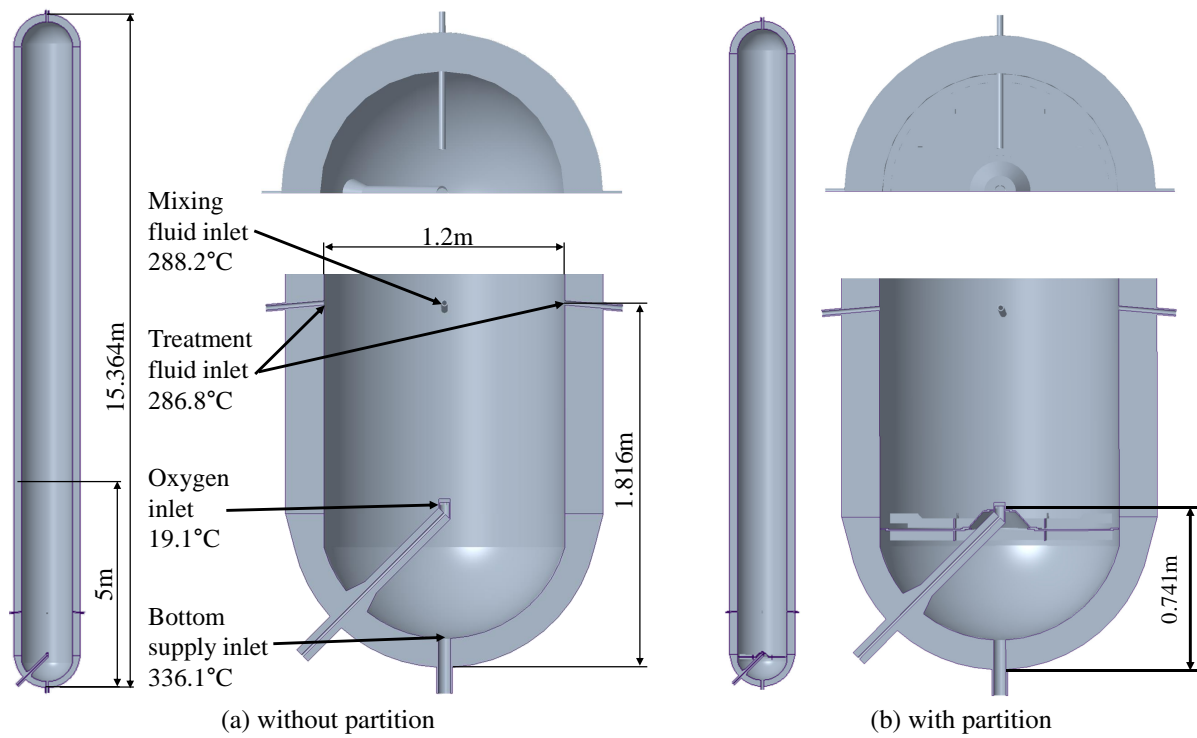
(a) without partition

(b) with partition

Figure 2: 3D solid model of hydrothermal destruction reactor vessel

(a-1) symmetrical plane   (a-2) cross section
(a) without partition, total 7,457,054 cells

(b-1) symmetrical plane   (b-2) cross section
(b) with partition, total 20,299,821 cells
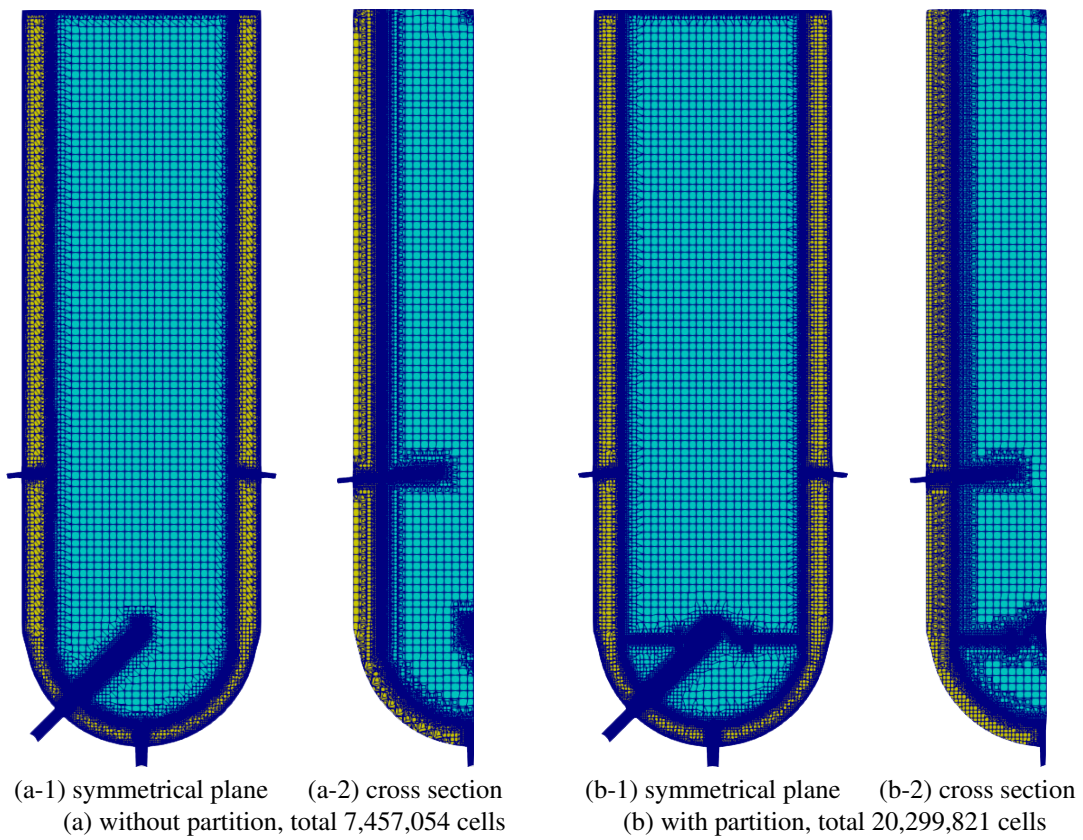
Figure 3: Finite volume mesh

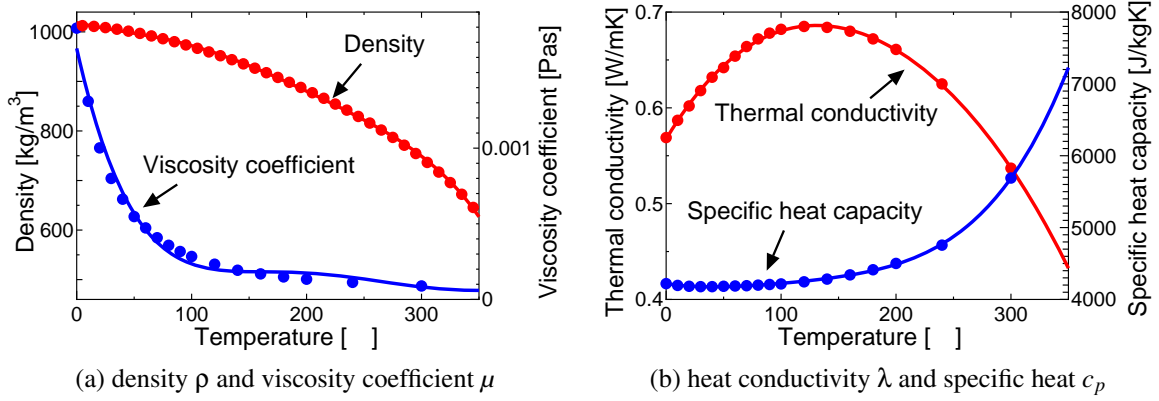(a) density ρ and viscosity coefficient μ (b) heat conductivity λ and specific heat c_p

Figure 4: Temperature dependent thermophysical properties of fluid

Table 1: Thermophysical properties of inconel alloy (NCF690, 20 °C)

Density ρ	8200 kg/m³
Specific heat c_p	450 J/(kg K)
Thermal conductivity λ	12 W/(m K)

Table 2: Boundary conditions

	Fluid region			Solid region
	Temperature [°C]	Velocity [m/s]	Pressure [MPa]	Temperature [°C]
Mixing fluid inlet	288.2	0.6950		288.2
Side wall of mixing fluid nozzle	288.2	non-slip		288.2
Treatment fluid inlet	286.8	0.6040		286.8
Side wall of treatment fluid nozzle	286.8	non-slip		286.8
Oxygen inlet	19.1	0.0467		19.1
Side wall of oxygen nozzle	19.1	non-slip		19.1
Bottom supply inlet	336.1	0.0176		336.1
Outlet (top surface)	369.9	uniform	26.5	369.9
Outer wall of vessel	—	—	—	insulation
Inner wall of vessel	heat transfer	non-slip		heat transfer
Bottom partition	heat transfer	non-slip		heat transfer

The analysis of half model of the reactor vessel is carried out considering symmetry structure. Two types of FVA models are constructed with and without the bottom partition to compare results.

Unstructured FVA mesh is generated using a standard meshing utility snappyHexMesh of the Open-FOAM based on 3D geometry data in the standard triangulated language (STL) format of the 3D solid vessel models. Figure 3 shows FVA mesh. In the figure, yellow and light blue cells represent solid and fluid regions, respectively.

3.2 Thermophysical properties and boundary conditions

In order to express temperature dependence of the thermophysical properties of the internal fluid, density ρ [kg/m^3], viscosity μ [Pa s], thermal conductivity λ [W/(m K)], and specific heat c_p [J/(kg K)] are approximated by polynomial equations of temperature T [K],

$$f(T) = \sum_{i=0}^{N} a_i T^i \tag{7}$$

as shown in Fig. 4, where N is degree of the polynomial, $a_0, a_1, \ldots, a_N$ are coefficients and are calculated by least squares approximation. For the heat conduction analysis of the vessel body, temperature independent thermophysical properties of inconel (NCF690) are shown in Table 1.

Boundary conditions of multi-regionally coupled analysis are summarized in Table 2. At each inlet of the fluid region, temperature and flow velocity are set based on the measured values during actual operation of the reactor. Since the oxygen nozzle has a double circular structure and is constantly cooled by cooling water, temperature on the side wall of the nozzle is set to 19.1 °C. At the outlet, which is the top surface of the FV models, pressure is set to 26.5 MPa due to the measured value inside the actual vessel, and the uniform velocity outlet condition is configured. In addition, the outlet temperature is set to 369.9 °C, which is also the measured value, to simulate the heat generated by the chemical reaction in the hydrothermal oxidative decomposition of PCBs. On the outer wall of the vessel of solid region, heat transfer is insulated. The conjugate heat transfer is considered on the solid-liquid interface that are inner wall of vessel and surfaces of bottom partition.

4 RESULTS AND DISCUSSIONS

4.1 Temperature distribution

Figure 5 shows a comparison of the temperature distributions among the coupled analysis of thermal fluid and heat conduction, the thermal fluid analysis for the internal fluid, and the heat conduction analysis for the vessel body. In all analysis results, the top surface is uniform 369.9 °C, which is the temperature inside the actual vessel. The oxygen nozzle is at the lowest temperature of 19.1 °C, which has a cooling effect on bottom of the vessel.

Comparing the temperature distribution results at the bottom of the vessel, the results of the thermal fluid analysis for the internal fluid is the lowest temperature, and the heat conduction analysis for the vessel body is the highest temperature. In the thermal fluid analysis for the internal fluid, since the solid-liquid interface acts heat insulation, the temperature is reduced by the descent of the fluid cooled by the oxygen nozzle. The heat conduction analysis of the vessel body retains the hot water temperature at the inlet of the bottom. In contrast, the results of the coupled analysis are distributed between the temperatures of the other two results because of the heat transfer on the solid-liquid interface.

As shown in Fig. 5 (b), since heat conduction does not occur across partition in the thermal fluid analysis, the temperature differs significantly between top and bottom of the partition. The results of the coupled analysis show that the temperature in the lower region of the bottom partition is lower than without the partition because advection is blocked by the bottom partition.

Figure 6 shows comparisons of temperature distributions on the solid-liquid interface along a path from the center of the vessel bottom to the side wall on the symmetry plane opposite the oxygen nozzle as
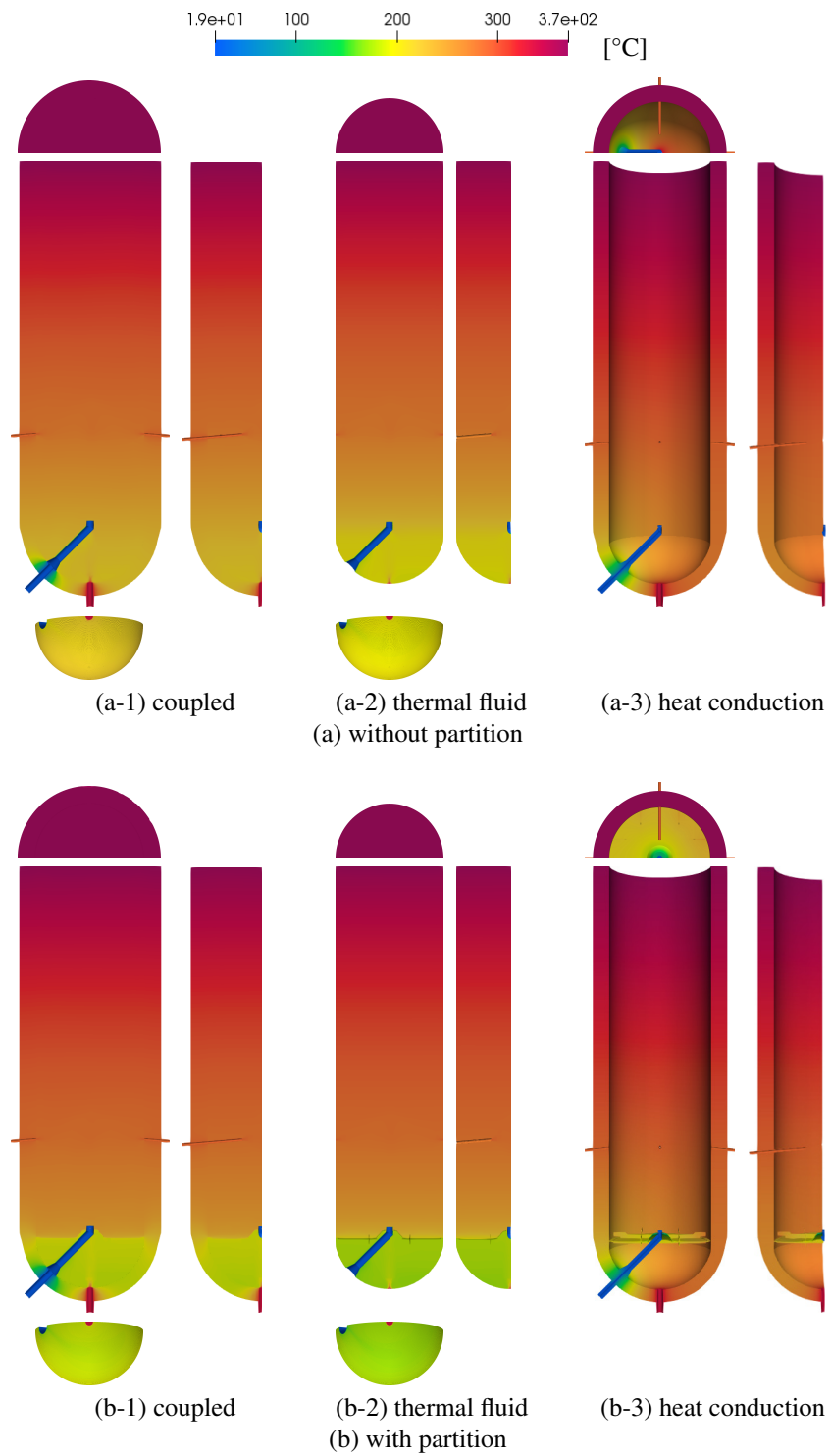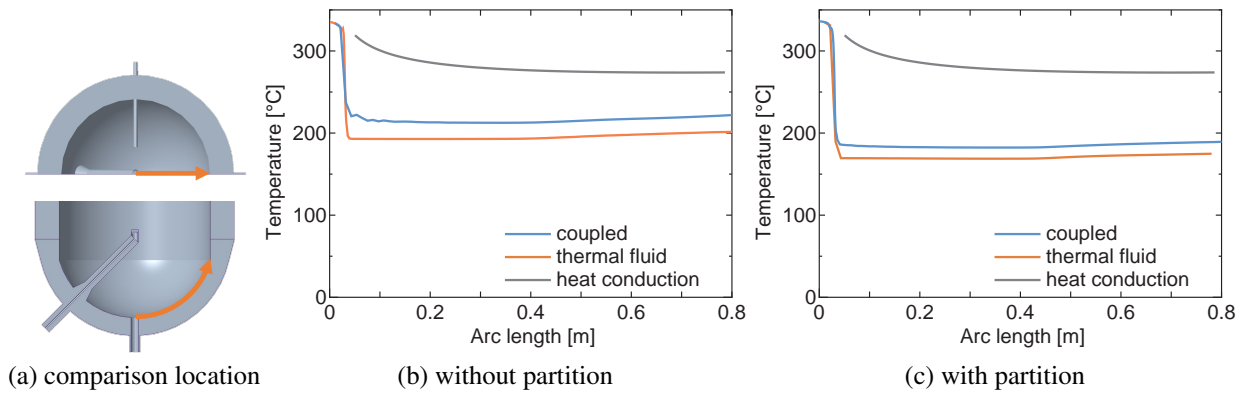
(a-1) coupled   (a-2) thermal fluid   (a-3) heat conduction

(a) without partition

(b-1) coupled   (b-2) thermal fluid   (b-3) heat conduction

(b) with partition

Figure 5: Temperature distribution

(a) comparison location   (b) without partition   (c) with partition

Figure 6: Temperature comparison at bottom of the vessel

(a-1) coupled   (a-2) thermal fluid   (b-1) coupled   (b-2) thermal fluid

(a) without partition   (b) with partition
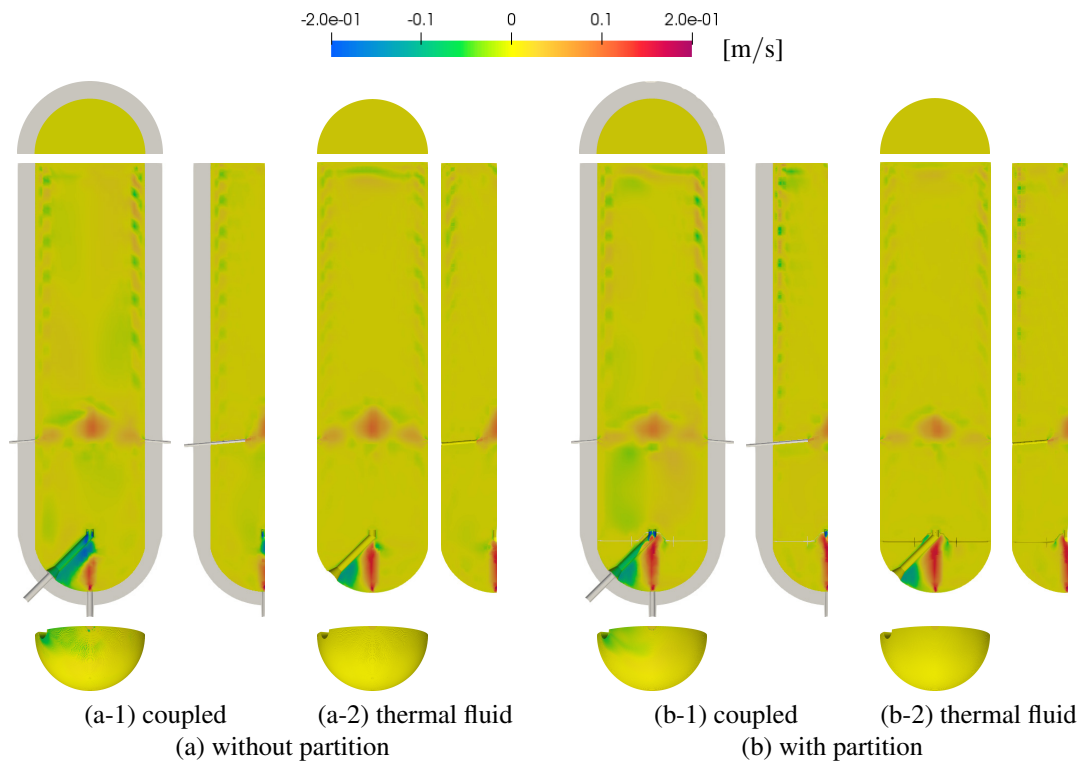
Figure 7: Velocity distribution in the vertical direction

(a-1) coupled   (a-2) thermal fluid   (b-1) coupled   (b-2) thermal fluid

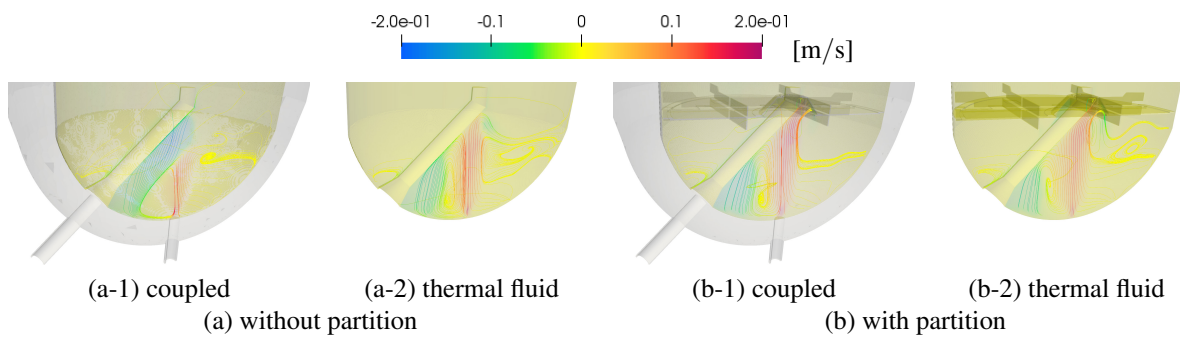(a) without partition   (b) with partition

Figure 8: Stream line

8

indicated by the orange line in Fig. 6 (a). With or without the bottom partition, the heat conduction analysis results of the vessel show higher temperature than the others because there is no advection by liquid oxygen and the fluid cooled by the oxygen nozzle. The results of the coupled analysis are higher than those of the thermal fluid analysis because of heat conduction in the vessel body.

4.2 Velocity distribution

The velocity distribution in the vertical direction which is height direction of the vessel is shown in Fig. 7 in comparison with the coupled analysis and the thermal fluid analysis. The outlet on the top surface has a uniform flow velocity, which is $0.001\,29\,\mathrm{m/s}$ in the vertical direction. The actual average flow velocity $3\,\mathrm{m/h} = 0.000\,83\,\mathrm{m/s}$ for the entire reactor of height $15\,\mathrm{m}$ with an in-vessel processing time of $5\,\mathrm{h}$ is similar order as the result around the top surface. In the bottom of the vessel, the fluid is cooled by the oxygen nozzles and is descended, and the hot water from the bottom inlet flows upward in both analysis results. In the coupled analysis, the downward flow is more extensive because the temperature between the oxygen nozzle and bottom of the vessel is larger than in the thermal fluid analysis.

Streamlines at the bottom of the vessel are shown in Fig. 8. The streamline color indicates the vertical flow velocity. The bottom supply inlet flow rises hot water flowing but the fluid is fallen down by the oxygen nozzle cooling, then causing circulation. In coupled analysis, the downward flow is larger than the thermal fluid analysis.

5 CONCLUSIONS

In this study, multi-regionally coupled analysis of thermal fluid for the internal fluid and heat conduction analysis for the vessel body is performed for hydrothermal oxidative destruction reactor of PCBs. It is considering the heat transfer on the solid-liquid interface. The heat generation of the chemical reaction inside the reactor is introduced by setting the temperature boundary condition as measured during the actual operation. The effect of the coupled analysis is clarified by comparing the results with and without the bottom partition, and the coupled analysis with the uncoupled analyses.

ACKNOWLEDGMENT

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[2] OpenFOAM (Free CFD Software) The OpenFOAM Foundation, https://openfoam.org/