

Effect of Structure Deformation on Mechanical Energy Generation

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ABSTRACT

This paper proposes a novel methodology to incorporate structural deformation effects directly into the pressure iteration scheme of the SIMMER-III code for mechanistic analysis of post-disassembly expansion (PDE) phase in sodium-cooled fast reactors (SFRs).

In the core disruptive accidents of SFRs, prompt criticality may generate substantial thermal energy, leading to the expansion of high-pressure core material. The associated mechanical energy generation during the PDE phase challenges reactor vessel integrity. Conventional approaches analyze vessel integrity through transferring SIMMER-derived mechanical energy to structural codes such as AUTODYN. However, these methods introduce uncertainties when converting SIMMER-derived mechanical energy into structural loading conditions. Moreover, an attempt to couple SIMMER-III with structural code with explicit coupling methods may introduce numerical instability and cannot fully capture fluid–structure interaction effects.

The present study resolves this limitation by embedding structure deformation implicitly into SIMMER's semi-implicit pressure solver. Instead of explicit fluid–structure coupling, the structure deformation-induced volume change is reformulated as a modification of the effective bulk modulus of sodium within each finite-differencing cell. Validation using a single-phase sodium shock tube demonstrated accurate prediction of pressure wave propagation velocity, consistent with theoretical solutions, and without numerical instability. The method was applied to PDE analysis of the ESRF-SMR concept. Results indicate that redan wall deformation alters local pressure wave propagation and damping characteristics but has limited impact on peak mechanical energy generation. Nevertheless, the proposed approach eliminates coupling uncertainties and establishes a foundation for fully integrated fluid–structure interaction analysis in SFR severe accident assessment.

KEYWORDS

SFR, CDA, SIMMER, PDE, STRUCTURE DEFORMATION

1. INTRODUCTION

As the fast reactor core is not configured to maximize reactivity, a core disruptive accident (CDA) has the potential to cause a rapid increase in reactor power due to prompt criticality. This generates large amounts of thermal energy and produces high-temperature, high-pressure core material. The generation of excessive energy due to prompt criticality is known as energetics, and is considered one of the major issues in the safety of fast reactors. The core material, heated and pressurized by the energetics, expands to the cover gas volume within a few hundred milliseconds. This process of core material expansion converts thermal energy into mechanical energy, which may affect the integrity of the reactor vessel and primary coolant system. This process is known as the post-disassembly expansion (PDE) phase. The integrity of the primary coolant boundary and the extent of sodium leakage in this phase are key considerations in the safety assessment of fast reactors.

In the early stages of fast reactor development, the isentropic expansion potential (IEP) of the fuel to atmospheric pressure was used to evaluate the mechanical energy generated in the PDE phase [1, 2]. This evaluation is overly conservative since the IEP is merely a thermodynamic upper limit of mechanical energy in the fuel expansion, and it neglects the inherently available mechanisms that limit the generation of mechanical energy. These are: temperature homogenization due to the mixing of core material within the core; thermal and hydraulic losses when the material is discharged through the upper core structure; and condensation of vapor when the material expands into the upper sodium plenum region. Furthermore, as the generation of mechanical energy is driven by the pressure of sodium vapor produced by fuel-coolant interaction (FCI), where high-temperature core material comes into contact with sodium, it is inappropriate to use the IEP of the fuel as an indicator of mechanical energy. For this reason, the SIMMER-III code [3, 4] was developed as a method of mechanistic analysis of the processes, such as core material expansion and discharge through the upper core structure (UCS), FCI between core material and sodium, and the growth of sodium vapor bubble, also known as the CDA bubble. The SIMMER-III code has been applied to the evaluation of mechanical energy in various SFRs [5-7].

The integrity of the reactor vessel against mechanical energy is evaluated using structural analysis codes such as AUTODYN [8] and EUROPLEXUS [9]. These codes analyze the interaction between single-phase sodium flow and structure deformation. In order to simulate the growth of a CDA bubble in these analysis codes, it is necessary to provide information on the pressure change according to the expansion of CDA bubble, either as a polytropic exponent [10] or as the relationship between bubble volume and pressure (P- ΔV curve) [11], in addition to the initial pressure of the bubble. This leads to uncertainty in the conversion of the mechanical energy evaluated by SIMMER-III into the parameters of these bubble growth behaviors. In addition, the growth of CDA bubble and the deformation of the reactor vessel occur simultaneously and the reactor vessel deformation may affect the growth of CDA bubble in reality. This effect cannot be taken into account if the subsequent analyses of mechanical energy and structure deformation are conducted sequentially by SIMMER-III and structural codes, respectively. For this reason, an attempt had been made to develop an evaluation method that combines SIMMER-III with the finite element method, which analyzes structural deformation in the past [12]. However, it had limitations in numerical stability, since the method of linking SIMMER-III with the structural deformation analysis code was performed by the explicit transfer of pressure and structure deformation amounts. Therefore, this study proposes a method to directly incorporate the effect of structure deformation into the pressure iteration performed in the semi-implicit fluid dynamics algorithm in SIMMER-III. The newly proposed method is applied to the PDE analysis of the ESFR-SMR [14] reactor and the effect of structure deformation on the mechanical energy generation is investigated.

2. STRUCTURE DEFORMATION MODEL FOR SIMMER

During the PDE phase, single-phase pressure peaks of several MPa are generated in the upper sodium plenum. The structure deformation of reactor vessel due to these single-phase pressure peaks is expected to be on the order of several millimeters to several centimeters. To analyze the structure deformation caused by the pressure transient in single-phase liquid, it is necessary to implicitly couple the effect of the structure deformation in the semi-implicit pressure iteration of SIMMER-III, since single-phase pressure changes significantly with the slight deformation of structure. Otherwise, the inconsistency between the pressure iteration and the volume change of single-phase liquid in the finite differencing cell due to structure deformation results in unphysical and/or unstable pressure prediction. On the other hand, if the cell is a gas-liquid two-phase system, the effect of structure deformation on the two-phase pressure within the cell is small, so explicit coupling between the structure deformation and SIMMER is sufficient and such implicit coupling is unnecessary. The structure deformation is usually analyzed by computer codes using finite element method with Lagrangian mesh and SIMMER-III uses finite differencing method with Eulerian mesh. The implicit coupling of these codes requires tedious and complicated geometrical procedure which makes this implicit coupling difficult. Therefore, this study proposes new method to couple the structure deformation and the pressure iteration in SIMMER-III. The idea is to regard the change of volume fraction of single-phase liquid sodium by structure deformation as the change of the pressure derivative of specific volume of sodium that is used in pressure iteration. This means that the change in the volume of single-phase sodium due to structure

deformation is instead considered to be a change in the compression of the single-phase sodium without changing the mass of sodium in a finite differencing cell.

2.1 Overview of SIMMER-III

The SIMMER-III code [3,4] is a computational code that performs a comprehensive analysis of the neutronic and thermal-hydraulic behavior of a damaged SFR core. The SIMMER code is employed to analyze the propagation of the disrupted area within the reactor core and the consequent reactor power transients in the CDAs of SFR, with a particular focus on the energy generation behavior due to prompt criticality and the transformation of this energy into mechanical energy by core expansion in the PDE phase. The code incorporates a fluid dynamics module to calculate thermal hydraulics of the mixture of degraded core materials, a neutronics calculation module to analyze space-dependent reactor kinetics, and a structure module that considers the melting and failure of structures such as fuel pins and wrapper tubes. SIMMER treats core materials such as fuel, steel, sodium, and fission gas as different components in solid, liquid, and gaseous states. The fluid dynamics module computes multi-velocity-field, multi-phase, multi-component flow, heat and mass transfer between components, and momentum exchange. As shown in Figure 1, SIMMER has three structural components in a finite difference cell to model the fuel subassembly of SFR. These components are the left can wall (LCW), the right can wall (RCW), and the pin. Since the reactor vessel is typically modeled using RCW, we developed a method that assumes the RCW deforms due to pressure change within the cell.

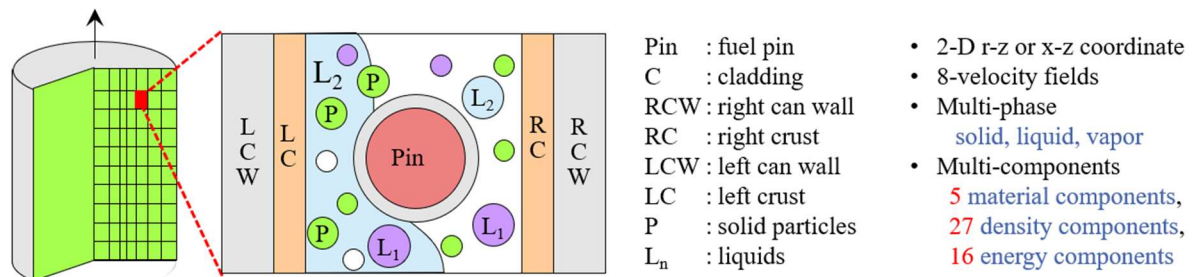


Figure 1: Conceptual figure of finite differencing cell in SIMMER-III

2.2 Method to Couple Structure Deformation with Pressure Iteration in SIMMER-III

Assume a finite differencing cell in two-dimensional cylindrical coordinate with a base area of A_c and RCW of its thickness w in SIMMER-III. The height of the cell is Δz , the radius of the cell right boundary is R and the circumferential cell width is $2\pi R$ as shown in Figure 2. The volume in the cell other than RCW is occupied by single-phase liquid sodium.

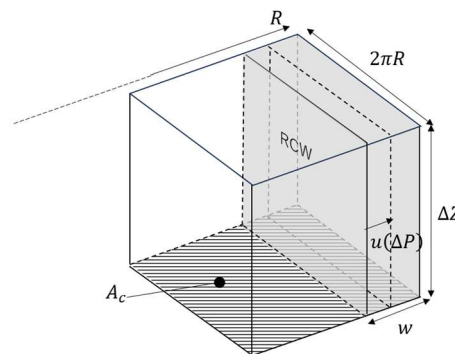


Figure 2: Conceptual schematics of finite differencing cell with RCW

The volume of the cell, the concentric RCW cylinder and the single-phase liquid sodium in the

cell are given by

$$V_c = A_c \Delta z \quad (1)$$

$$V_{RCW} = \pi w(2R - w) \Delta z \quad (2)$$

$$V_s = V_c - V_{RCW} \quad (3)$$

Consider a situation where the pressure in the cell increases by ΔP and the RCW deforms to the right and/or outer direction by $u(\Delta P)$. If the RCW does not deform, the change of sodium volume ΔV_s in the cell due to the pressure increase is given by the following equation:

$$-K \frac{\Delta V_s}{V_s} = \Delta P \quad (4)$$

where K is the bulk modulus of sodium. When the RCW deforms to the right direction by $u(\Delta P)$, the volume of the concentric cylinder, which is created by this deformation, can be regarded as the excessive volume change using effective bulk modulus, which takes RCW deformation into account. This is expressed by the following equation:

$$-\tilde{K} \frac{\Delta V_s - \pi u(\Delta P)[2(R - w) + u(\Delta P)] \Delta z}{V_s} = \Delta P \quad (5)$$

where $\tilde{K}$ is the effective bulk modulus of sodium taking the effect of RCW deformation into account. Note that ΔV_s is negative and $u(\Delta P)$ is positive for positive ΔP . Therefore, the sign of the second term in the numerator on the left-hand side of equation (5) is minus. Combining these two equations, the following equation holds:

$$\tilde{K} = \left\{ \frac{\Delta V_s - \pi u(\Delta P)[2(R - w) + u(\Delta P)] \Delta z}{\Delta V_s} \right\}^{-1} K \quad (6)$$

Substituting equations (2), (3) and (4) into equation (6) and rearranging gives the following equation:

$$\tilde{K} = \left\{ 1 + \frac{2\pi(R - w) \cdot u(\Delta P)}{\Delta P[A_c - \pi w(2R - w)]} K \right\}^{-1} K \quad (7)$$

where $O[u(\Delta P)^2]$ is neglected. Structural analysis codes provide $u(\Delta P)$. However, for implicit coupling with the pressure iteration in the SIMMER code, structural analysis codes need to provide the derivative of wall displacement with respect to pressure, not the displacement. Then, $u(\Delta P)$ is given by the following equation:

$$u(\Delta P) = \left(\frac{dw}{dP} \right) \Delta P \quad (8)$$

Substituting eq. (8) into eq. (7) and using the definition of bulk modulus,

$$K = - \frac{v_L}{\left(\frac{dv_L}{dp} \right)} \quad (9)$$

The following equation is obtained:

$$\left(\frac{d\widetilde{v_L}}{dp}\right) = \left(\frac{dv_L}{dp}\right) - \frac{2\pi(R-w)}{[A_c - \pi w(2R-w)]} \left(\frac{dw}{dP}\right) v_L \quad (10)$$

Equation (10) is the effective pressure derivative of the sodium-specific volume, taking into account the RCW deformation. This derivative is used in the pressure iteration in SIMMER-III instead of the original derivative.

Here, instead of receiving $u(\Delta P)$ from structural analysis codes, theoretical solution of $u(\Delta P)$ for elastic deformation is used to confirm the validity of the proposed method by simple test calculation. The elastic deformation of thick cylinder wall at the wall inner surface is given by:

$$u(\Delta P) = \frac{\Delta P}{E(1-n^2)} [(1-\nu)n^2 + 1 + \nu](R-w) \quad (11)$$

where E is Young's modulus, ν is Poisson ratio, and $n = 1 - w/R$. Using equation (11) instead of equation (8) gives the following equation:

$$\left(\frac{d\widetilde{v_L}}{dp}\right) = \left(\frac{dv_L}{dp}\right) - \frac{2\pi[(1-\nu)n^2 + 1 + \nu](R-w)^2}{[A_c - \pi w(2R-w)]E(1-n^2)} v_L \quad (12)$$

2.3 Test Calculation of single-phase shock tube

In order to validate the proposed method, the change of pressure wave propagation speed in a tube by wall deformation was analyzed using equation (12). As shown in Figure 3, shock tube with inner diameter of 10 cm, length of 1 m, and wall thickness of 5 mm is filled with single-phase liquid sodium at a temperature of 810 K and an initial pressure of 0.1 MPa. The pressure at one end is increased to 1.0 MPa suddenly and kept. First, the analysis was performed without the pipe wall deformation using one dimensional analysis arrangement with 100 cells. Pressure wave propagates and reflects at another end as shown in Figure 4 (a), which shows the pressure distribution along with the shock tube. This figure confirms that SIMMER-III properly analyzes the pressure wave propagation in the single-phase shock tube. The first arrival of pressure wave to the opposite end is evaluated as 0.442 ms, where the pressure at the end reaches the average of 0.1MPa and 1.0 MPa as shown in this figure. The sound velocity is evaluated to be $1/0.000442 = 2262.4$ m/s. Then, the analysis with wall deformation was performed. The theoretical sound velocity with wall deformation $\tilde{c}$ is given by the following equation [13]:

$$\tilde{c} = \left(\frac{1}{c^2} + \frac{D}{Et v_L} \right)^{-\frac{1}{2}} \quad (13)$$

where c is the sound velocity without wall deformation, D is wall diameter and t is wall thickness. Substituting D , t , $E = 1.93 \times 10^{11}$ Pa and $v_L = 1.223 \times 10^{-3}$ m³/kg, the sound velocity becomes $\tilde{c} = 1889.6$ m/s and the arrival time is estimated to be 0.530 ms. Figure 4 (b) shows the calculated shock wave propagation with wall deformation using equation (12). It is noteworthy that no numerical instability is observed, despite the structural deformation being considered. The calculated arrival time is 0.533 ms, which is in good agreement with the theoretical prediction. This confirmed that the newly developed method analyzed the effect of pipe deformation by pressure wave properly.

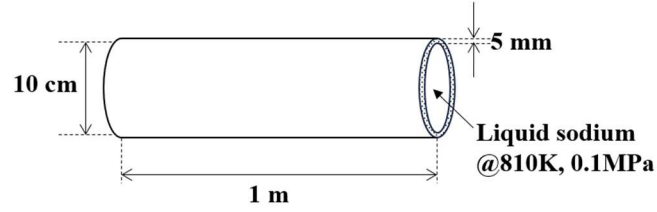


Figure 3: Shock tube filled with single phase sodium

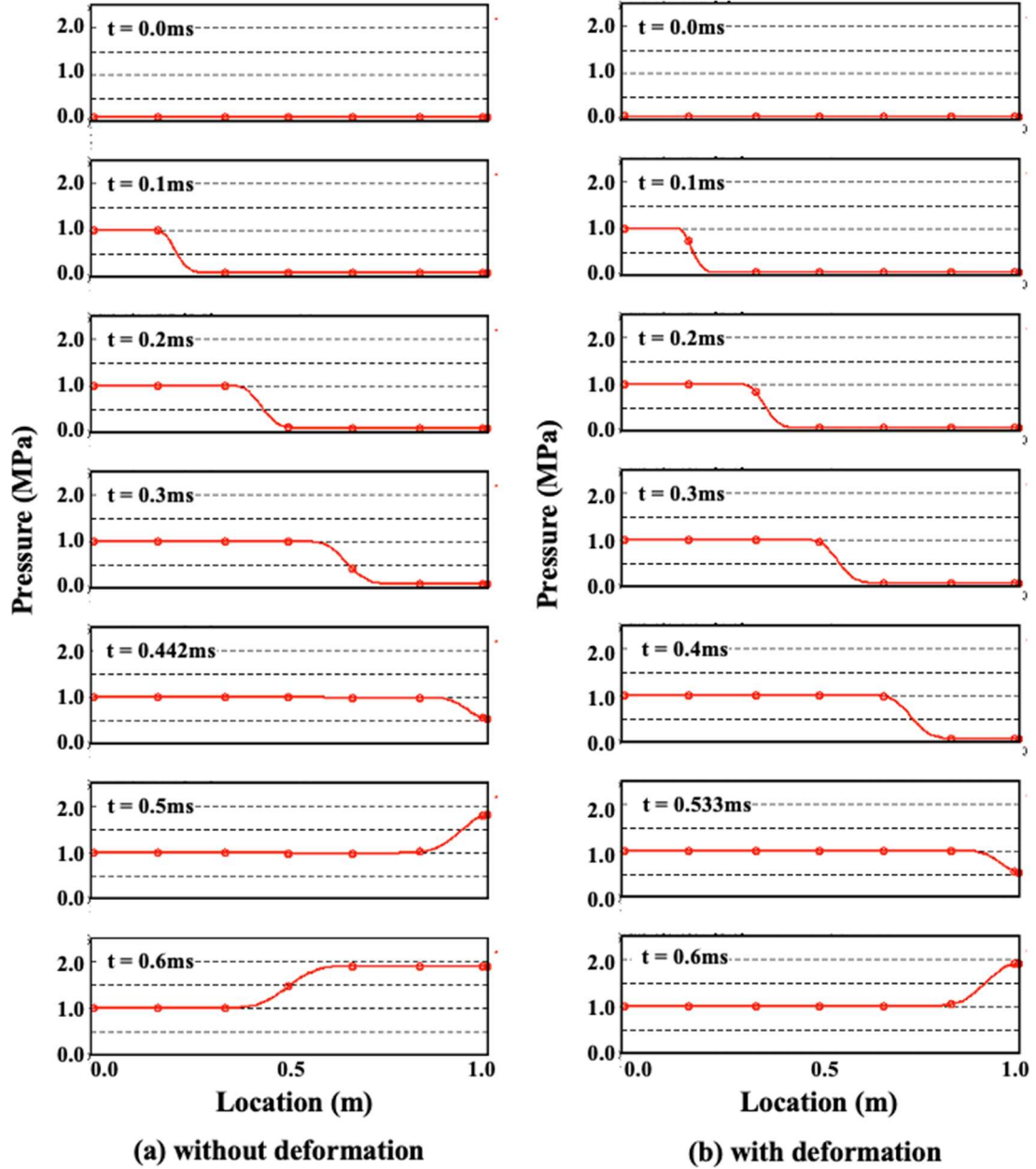


Figure 4: Pressure wave propagation in shock tube without/with wall deformation

3. APPLICATION TO THE ANALYSIS OF PDE PHASE

The proposed method was applied to the analysis of the PDE phase in the ESFR-SMR reactor [14] using equation (12). Figure 5 shows the analytical arrangement of the PDE phase analysis of ESFR-SMR. The core materials, sodium coolant and structures above the bottom of reactor core are modelled

in a cylindrical two-dimensional system using SIMMER-III as shown in this figure. EFR-SMR has a reactor vessel with a radius of about 4.5 m, and a redan wall with a radius of about 4.1 m exists inside the reactor vessel. The thickness of redan wall is about 2.5 cm. In this analysis, the deformation of the redan wall due to the pressure transient and its influence to the PDE phase are analyzed. The distribution of material and temperature in the fuel assembly just after prompt criticality was transferred from the transient phase analysis [15] to this analytical arrangement. The average and the maximum fuel temperature are 4128K and 5625K, respectively. The isentropic expansion potential of fuel to atmospheric pressure is 276MJ.

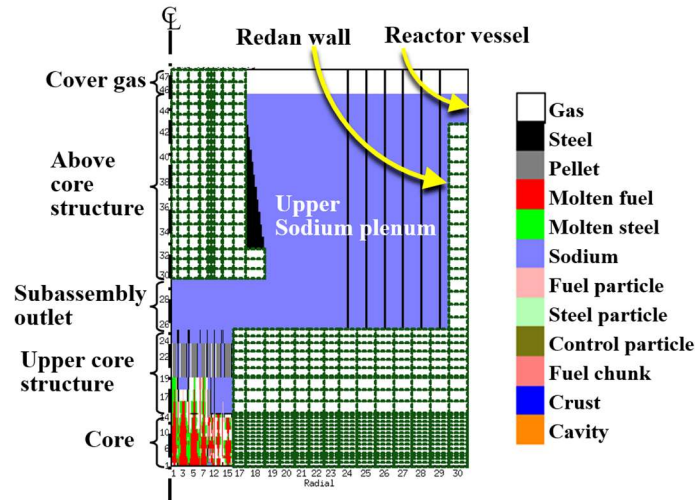


Figure 5: Analytical arrangement of PDE analysis of EFR-SMR using SIMMER-III

The high-temperature, high-pressure core material expands and moves upward from core region to upper core structure (UCS) region, and finally to subassembly (SA) outlet region. During this process, the core material undergoes fuel coolant interaction (FCI) with the sodium in these regions. The FCI generates sodium vapor, which forms a large vapor bubble (CDA bubble) at the bottom of the upper sodium plenum in the reactor vessel. The growth of the CDA bubble accelerates the sodium in upper sodium plenum upward, generating mechanical energy that may affect the integrity of the reactor vessel and primary coolant system.

Figure 6 gives the calculated transient of mechanical energy up to 3 seconds in both cases with and without redan wall deformation. “Kinetic energy” is the kinetic energy of sodium, “CG compress” is the compression work of cover gas, “Potential energy” is the gravitational potential energy of sodium and “Mechanical energy” is the sum of these energy components. After several cycles of the generation of mechanical energy due to the growth of CDA bubble and its shrinkage by condensation, the temperature of the core material finally lowers and the growth of CDA bubble hardly occurs after about 2 seconds. In both cases, the maximum mechanical energy is generated during the first growth of CDA bubble. It reaches a maximum value of 8.6 MJ at 64 ms in the case without wall deformation and 9.0 MJ at 68 ms in the case with wall deformation. Although the first mechanical energy peak is the largest, the mechanical energy generated after the second CDA bubble expansion cannot be ignored. The reason for this multiple growth of CDA bubbles and the generation of mechanical energy is that, as the bubble grows, the inertia of the sodium slug and the condensation of sodium steam in CDA bubble reduce the bubble pressure. This causes the hot core material to move from the core to the center of the CDA bubble, then the shrinkage of the bubble causes FCI again.

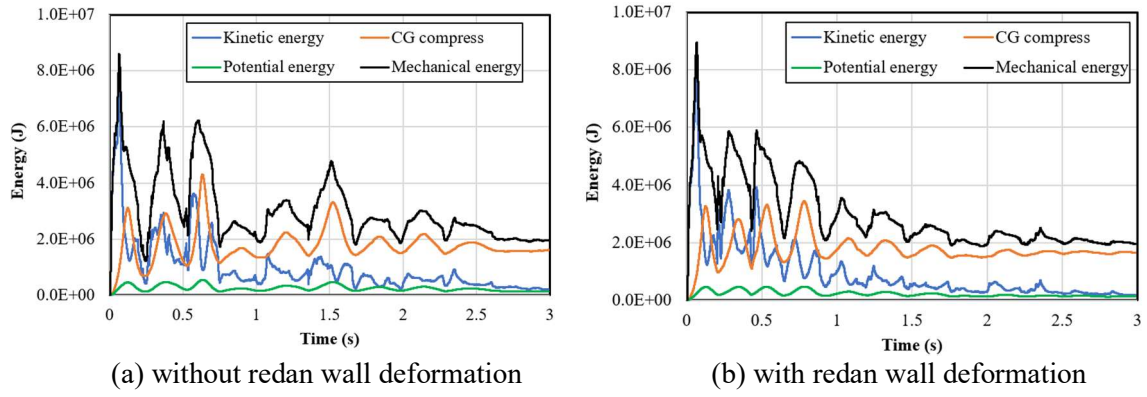


Figure 6: Transients of mechanical energy

The effect of wall deformation appears in the pressure wave propagation during the growth of the CDA bubble. Figure 7 shows the pressure contour map of the upper sodium plenum, the pressure transient at the lower-right corner of the upper sodium plenum, and the time transient of mechanical energy for these two cases. The pressure contour map shows the pressure distribution when the pressure at the lower-right corner of the upper sodium plenum reaches its maximum value. The CDA bubble takes approximately 80 ms to grow and generate mechanical energy. During this time, single-phase pressure wave propagates and reflects multiple times inside the upper sodium plenum. This produces oscillating pulse in the pressure. When wall deformation is not considered, this oscillation has time intervals of several milliseconds as shown in Figure 7 (a). However, when wall deformation is considered, the single-phase pressure is absorbed by the wall deformation, increasing the time interval to approximately 20 milliseconds as shown in Figure 7 (b). The pressure contour map also shows that the single-phase pressure in the upper sodium plenum is absorbed by the wall deformation. However, the difference in the propagation behavior of this single-phase pressure wave does not significantly affect the macroscopic behavior of the CDA bubble growth and mechanical energy generation.

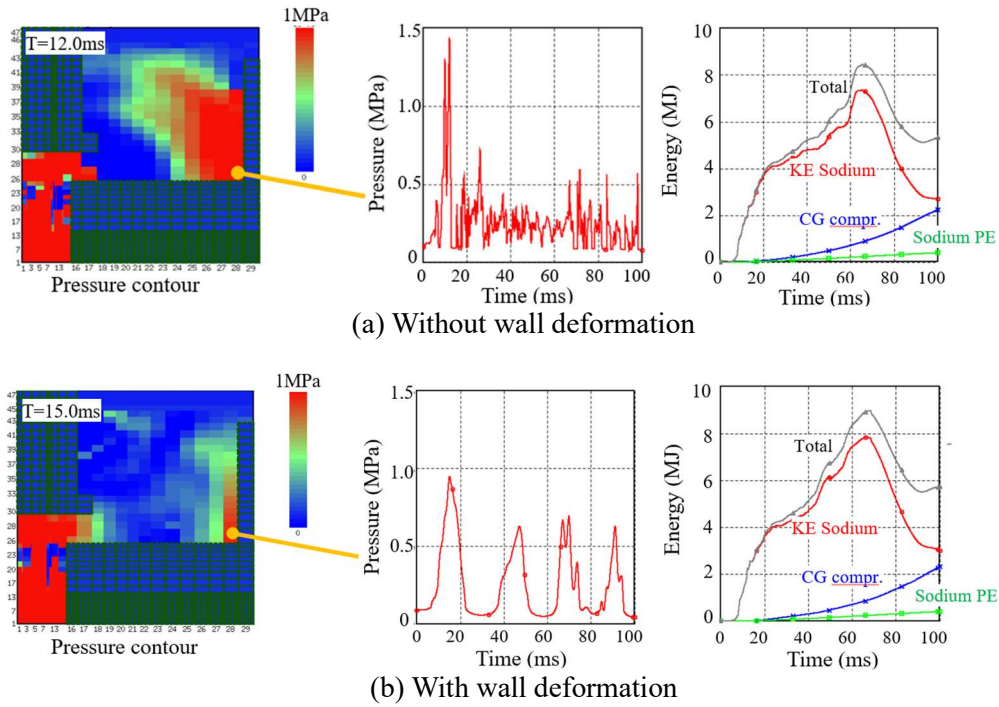


Figure 7: Propagation of pressure wave during CDA bubble growth

Currently, the structural analysis code and SIMMER are not coupled, therefore this analysis was performed using equation (12), as mentioned above. As Figure 7 shows, the maximum pressure on the redan wall surface is less than 1.5 MPa, and the deformation of the redan wall falls within the elastic deformation range assumed in equation (12). Figure 8 shows the axial pressure distribution along the redan wall at 12.0 ms, when the pressure at the bottom of the redan wall is at its maximum value in Figure 7(a). Pressure is highest at the bottom of the redan wall, decreasing upwards, and is approximately equal to the cover gas pressure above about two-thirds of the height of the upper sodium plenum. Since equation (12) ignores the axial effect, it is thought that the calculated deformation in the high-pressure region in Figure 8 is overestimated. However, this overestimation of deformation does not affect the conclusion that the impact of reactor vessel deformation on mechanical energy generation is small. Consideration of plastic deformation, axial effects and three-dimensionality by the coupling with structure analysis code will remain as a challenge in the future. Note that numerical stability will be guaranteed in this coupling by the use of equation (10).

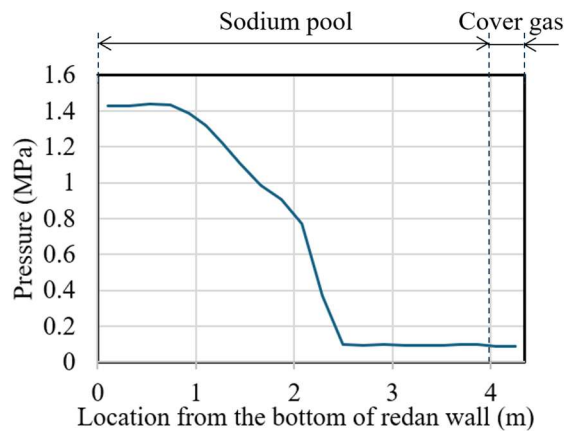


Figure 8: Pressure distribution along the redan wall

4. CONCLUSIONS

This study developed a new method to directly incorporate the effect of structure deformation into the pressure iteration in the semi-implicit fluid dynamics algorithm in SIMMER-III. Validation using a single-phase sodium shock tube demonstrated accurate prediction of the change of pressure wave propagation velocity by the deformation of tube wall, consistent with theoretical solutions, and without numerical instability. The method was applied to the analysis of the PDE phase of ESFR-SMR. Results indicate that redan wall deformation alters local pressure wave propagation and damping characteristics but has limited impact on peak mechanical energy generation.

Nevertheless, this new method provides the first step towards developing a methodology that eliminates the uncertainties associated with the conventional methods, which connect SIMMER-III mechanical energy evaluations to structural analysis codes such as AUTODYN or EUROPLEXUS. Furthermore, the PDE analysis of ESFR-SMR in this study demonstrated that the growth of CDA bubbles and the generation of mechanical energy occurred multiple times. The development of a direct coupling method of structural deformation analysis with SIMMER-III based on the new method will make it possible to evaluate the integrity of the reactor vessel against the cumulative damage by these multiple energy generation events, which is difficult to achieve by the conventional methods. Overall, this study demonstrates a stable and physically consistent framework for future fully coupled fluid–structure interaction analyses using SIMMER-III and structural analysis codes in SFR severe accident assessment.

NOMENCLATURE

A_c : Base area of finite differential cell
 c : Sound velocity

$\tilde{c}$:	Sound velocity with wall deformation
D :	Diameter of pipe
E :	Young's modulus
K :	Bulk modulus of sodium
$\tilde{K}$:	Effective bulk modulus of sodium with wall deformation
n :	$1 - w/R$
ΔP :	Pressure change
R :	Radius of the right boundary of finite differential cell
t :	Thickness of pipe
u :	Deformation of structure
V_c :	Volume of finite differential cell
V_S :	Volume of sodium in finite differential cell
V_{RCW} :	Volume of right can wall in finite differential cell
w :	Thickness of right can wall
Δz :	Height of finite differential cell
ν :	Poisson ratio

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