

MODELING OF EVAPORATION PROCESSES UNDER THE GROUND

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ABSTRACT: The vaporization process is modeled by incorporating the relation between pressure and enthalpy into the numerical simulation code for the coupled thermal, hydraulic and mechanical phenomena under the ground. The boundary between superheated steam and two-phase of steam and water was modeled by the previous study. On the other hand, the boundary between compressed water and two-phase of steam and liquid is modeled by the deduced equation with pressure and enthalpy in this study. Temperature is selected to be the unknown variable in the model. The enthalpy is estimated from the pressure and temperature, and then the situation of phase is examined. As an example, the situation about the disposal of the waste generating heat to 300 °C is simulated by the simple 2-D and detail 1-D models.

Keywords: Groundwater, Evaporation, Coupled analysis, Nuclear Waste Disposal

1. INTRODUCTION

In Japanese nuclear energy policy, the high level radioactive waste from the nuclear fuel cycle is planned to be disposed in deep geology. The vitrified waste is stored for fifty years for cooling and then those are stored in overpack and disposed. This is because the stable and safe disposal is necessary. The plan, therefore, needs long time for disposal. However, since the accident at the nuclear plant Fukushima Daiichi, the disposal of nuclear waste requires urgent attention. If the nuclear fuel rod is directly disposed in the deep geology, the volume of waste may become very large and the heat generation from the waste is also very high. In this case, the effect of the high heat generation from the waste has to be examined and then repository has to be designed as most safe and stable as possible.

In this study, the vaporization process is modeled by incorporating the relation between pressure and enthalpy into the numerical simulation code for the coupled thermal, hydraulic and mechanical phenomena under the ground. The boundary between superheated steam and two-phase of steam and liquid was modeled by the previous study. On the other hand, the boundary between compressed water and two-phase of steam and water is modeled by the deduced equation with pressure and enthalpy in this study. In general, temperature is the unknown variable for the coupled problem and the boundary condition is given by temperature. Therefore, temperature is selected to be the unknown variable in the model. The enthalpy is estimated from the pressure and temperature, and then the situation of phase is examined. As an example, the situation about the disposal of the waste generating heat to 300 °C is simulated by the simple 2-D and detail 1-D model.

2. MODEL OF PHASE CHANGE

2.1 Pressure-enthalpy Diagram

Mercer and Faust [1] and White et al. [2] gave the diagram of phase change presented by pressure and enthalpy as shown in Fig.1. By using this diagram, the phase of fluid can be recognized. The bold convex line in the graph indicates the boundary of phases, in which the boundary between area ① and ② is the phase change between liquid and steam-liquid two phase, and that between ② and ③ is the one between steam-liquid two phase and superheated steam.

Although the diagram is the plane coordinate with the vertical axis of pressure and horizontal one of enthalpy, the isothermal line can be seen in the diagram. The phase change is originally explained by three dimensional diagram adding temperature as shown in Fig.2.

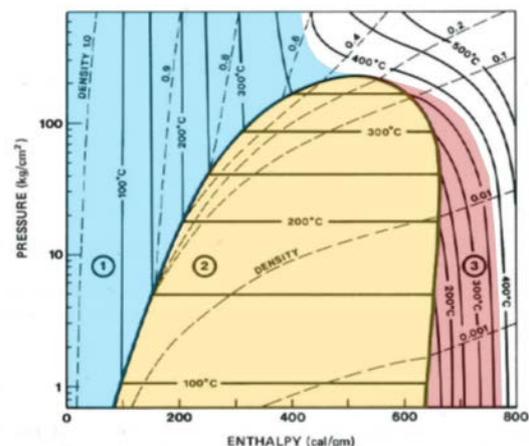


Fig.1 Pressure-enthalpy diagram for water and steam with thermodynamic regions [1], [2]

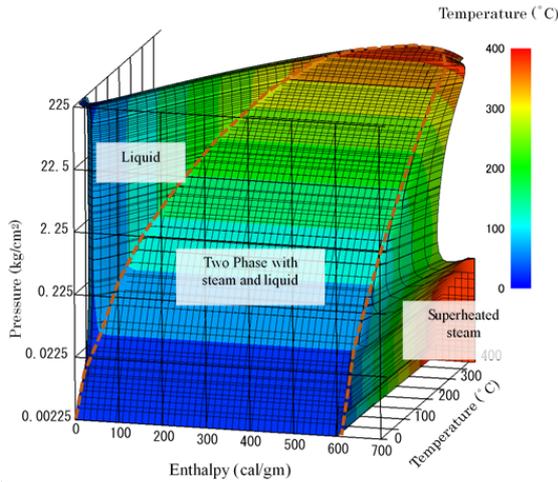


Fig.2 Pressure-enthalpy-temperature diagram for water and steam phases

2.2 Equation of Boundaries

The equation of boundary between ② and ③ in Fig.1 is given by Huyakorn and Pinder [3] as

$$h_*^g = 2822.82 - 39.952/p + 2.5434/p^2 - 0.93888p^2 \quad (1)$$

where h_*^g is the enthalpy (kJ/kg) at the boundary between two phase region and superheated steam, and p is the pressure (dyne/cm²). Temperature in the region ① at which enthalpy h is smaller than the enthalpy at the boundary between water and two phase region h_*^l is given by

$$T = \psi_1(p, h) + [\psi_0(p) - \psi_1(p, h_*^l)] \quad (2)$$

where

$$\psi_0(p) = 4667.075/(12.599 - \ln(10p)) - 273.15 \quad (3)$$

$$\psi_1(p, h) = -28.152 - 0.13746p + 0.30112h + \frac{3536.4}{h} - 4.3192 \times 10^{-5}h^2 \quad (4)$$

Temperature in the region ② where enthalpy h is between h_*^l and h_*^g is given as

$$T = \psi_0(p) \quad (5)$$

Temperature in the region ③ where enthalpy h is larger than h_*^g is obtained as

$$T = \psi_2(p, h) + [\psi_0(p) - \psi_2(p, h_*^g)] \quad (6)$$

in which

$$\begin{aligned} \psi_2(p, h) = & -374.67 + 47.992p - 0.63361p^2 \\ & + 7.3939 \times 10^{-5}h^2 \\ & - \frac{3.3372 \times 10^6}{p^2h^2}h^2 \\ & + \frac{0.035715}{p^3} - 1.1725 \\ & \times 10^{-9}h^3p - \frac{2.2686 \times 10^{15}}{h^4} \end{aligned} \quad (7)$$

As the boundary between liquid and two phase region was not given by Huyakorn and Pinder, the following equation is reduced in this study;

$$\begin{aligned} p^l = & -5 \times 10^{-11}h_*^l{}^5 + 4 \times 10^{-8}h_*^l{}^4 - 5 \times \\ & 10^{-6}h_*^l{}^3 + 0.0003h_*^l{}^2 + 0.0028h_*^l - 0.1422 \end{aligned} \quad (8)$$

Fig. 3 shows the fitting of Eqs. (1) and (8) to the steam diagram, from which it is understood that Eqs. (1) and (7) give the relatively good approximation.

In this study, the phase of fluid is examined by using the above relations.

3. GOVERNING EQUATIONS

3.1 Mass Conservation Law

The governing equation of seepage is given as

$$-\rho_w \frac{\partial \theta}{\partial \psi} \frac{\partial P}{\partial t} - [\rho_w k_{ij} P_{,j}]_{,i} = 0 \quad (9)$$

where θ is the volumetric moisture content, ψ is the matric potential, P is the total head, ρ_w is the density of water, k_{ij} is the hydraulic conductivity.

The density of water ρ^l (gm/cm³) is given as a function of pressure p and enthalpy h by Marcer and Faust,

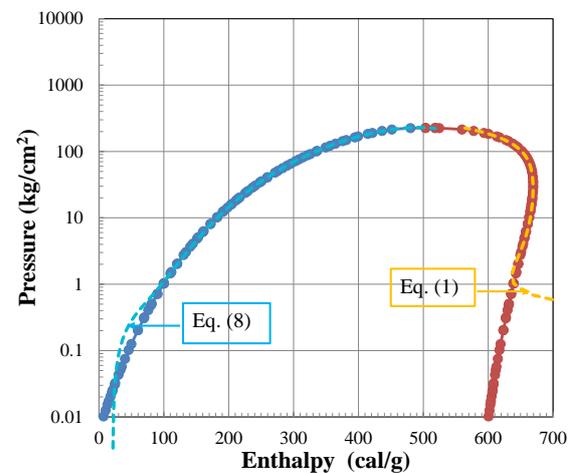


Fig. 3 Approximation relations and those fitting result

$$\rho^l = \begin{cases} 0.98988 + 4.0089 \times 10^{-4} p - 4.0049 \times 10^{-5} h + \\ 2.6661/h + 5.4628 \times 10^{-7} ph - 1.2996 \times 10^{-7} h^2 & \text{for } h > 200 \\ 1 & \text{for } h \leq 200 \end{cases} \quad (10)$$

The density of superheated steam ρ^g is given as

$$\rho^g = -2.2616 \times 10^{-5} + 0.043844 p - 1.7909 \times 10^{-5} ph + 3.6928 \times 10^{-8} p^3 + 5.1764 \times 10^{-13} ph^3 \quad (11)$$

The saturation degree of water S^l can be obtained by

$$S^l = \begin{cases} 1 & \text{for } h \leq h_s^l \\ 0 & \text{for } h \geq h_s^g \\ \frac{\rho^g (h_s^g - h)}{h(\rho^l - \rho^g) - (h_s^l \rho^l - h_s^g \rho^g)} & \text{for } h_s^l < h < h_s^g \end{cases} \quad (12)$$

The saturation degree of steam S^g is given by

$$S^g = 1 - S^l \quad (13)$$

The density of water ρ_w at the two phase of liquid and steam is given by

$$\rho_w = \rho^g S^g + \rho^l S^l = \rho^g (1 - S^l) + \rho^l S^l \quad (14)$$

On the other hand, the viscosity of water μ^l and that of steam μ^g are obtained as a function of temperature T by

$$\mu^l = 10^{-6} \times 239.4 \times 10^{[248.37/(T+113)]} \\ \mu^g = (0.407T + 80.4) \times 10^{-6} \quad (15)$$

in which the unit of the viscosity is g/(cm·s).

The relative permeability of water k_r^l and that of steam k_r^g are given as a function of saturation degree of water and steam as followings;

$$k_r^l = (S^l)^2 \\ k_r^g = (S^g)^2 = (1 - S^l)^2 \quad (16)$$

By using above parameters, the hydraulic conductivity tensor of water k_{ij}^l and that of steam k_{ij}^g is obtained by

$$k_{ij}^l = \frac{k_r^l \rho^l g K_{ij}}{\mu^l}$$

$$k_{ij}^g = \frac{k_r^g \rho^g g K_{ij}}{\mu^g} \quad (17)$$

The hydraulic conductivity in Eq. (9) is given by

$$k_{ij} = k_{ij}^l + k_{ij}^g = \left(\frac{k_r^l \rho^l}{\mu^l} + \frac{k_r^g \rho^g}{\mu^g} \right) g K_{ij} \quad (18)$$

where K_{ij} is the intrinsic permeability of the material. By applying the van Genuchten relation to the moisture capacity of the relation between θ and ψ , Eq. (9) can be solved by considering the situation of phase change of fluid.

3.2 Energy Conservation Law

The equation describing energy transport is written as

$$(\rho C)_m \frac{\partial T}{\partial t} + \{S_r \rho_w c_w v_i T - (\lambda_m)_{ij} T_{,j}\}_{,i} + \{L \rho_w dS^g\}_{,i} + Q^h = 0 \quad (19)$$

where

$$(\rho C)_m = n(S^l \rho^l C^l + S^g \rho^g C^g) + (1-n)\rho^s C^s \quad (20) \\ \lambda_m = n(S^l \lambda_m^l + S^g \lambda_m^g) + (1-n)\lambda_m^s$$

in which C^l is the specific heat of water and C^g is that of steam. λ_m^l is the thermal conductivity of water and λ_m^g is that of steam. Those are the function of temperature as shown in Fig. 4. Moreover, λ_m^s is the thermal conductivity of solid and n is the porosity.

L is the latent heat and dS^g is the change in saturation degree of steam. By solving Eqs. (9) and (19), total head P and temperature T are obtained. Then, the enthalpy is calculated by

$$h = E + p / \rho_w \quad (21)$$

E is the energy of the element and the second term is the pressure per unit weight (J/g or kJ/kg). The enthalpy and pressure is used to judge the phase situation.

4. SIMULATION EXAMPLES

4.1 2-D Model

4.1.1 Model Explanation

Fig. 5 shows the 2-D model of the situation around the waste in a repository. The horizontal length of the region is 36 m, the height is 29 m, waste is 1x1 m, tunnel with buffer material is 5x5 m and the

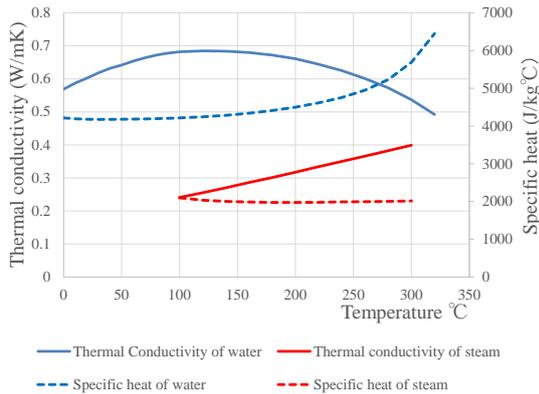


Fig.4 Nonlinear relation of thermal conductivity and specific heat to temperature

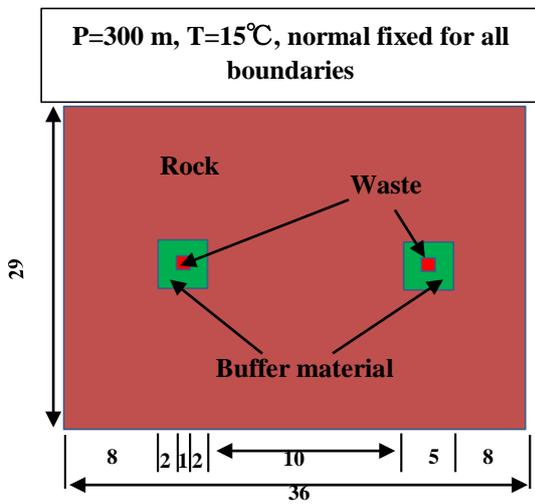


Fig. 5 Schematic view of 2-D model (unit: m)

distance between wastes is 14 m. The thermal initial condition is 15 °C and hydraulic one is 300 m for all region. As a boundary condition, normal deformation is fixed, total head is 300 m and temperature is 15 °C for all boundaries.

Fig. 6 shows the heat generation history at the waste. Temperature increases until 300 °C by 1 °C / 10days. Table 1 shows the parameters used in the analysis.

4.1.2 Analysis results of 2-D Model

Fig.7 shows the temperature distribution when temperature at waste becomes 300 °C. The rock between tunnels has temperature of over 120 °C. Fig. 8 shows the situation in the buffer material neighboring waste and rock and that in the rock neighboring buffer material when temperature at the waste reached 300 °C. The enthalpy in the buffer material neighboring waste is a little smaller than h^* and still evaporation does not occur. It is found that

the enthalpy becomes small with the distance from the waste. Fig. 9 shows the temporal change of relation between pressure and enthalpy in the buffer material neighboring waste. It is found that the pressure and enthalpy becomes gradually large and particularly the pressure raises to about 100 kg/cm²

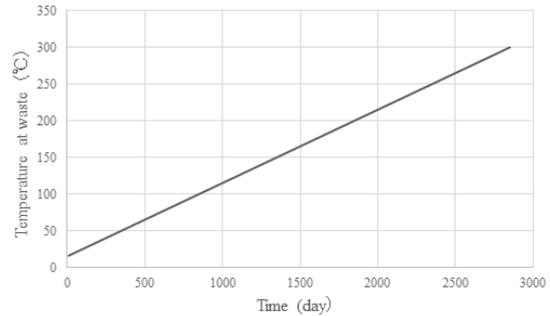


Fig.6 History of heat generation at the waste

Table 1 Parameters used in simulation

Parameter	Waste	Buffer	Rock
E (MPa)	2.00×10^5	3.44×10^1	1.82×10^3
ν	0.30	0.30	0.21
K (m)	1.0×10^{-30}	4.0×10^{-20}	1.3×10^{-15}
VG	θ_s	0.0001	0.403
	θ_r	0.0	0.0
	α	8.0×10^{-3}	8.0×10^{-3}
n	1.60	1.60	1.13
λ_f (J/(kg °C))		0.60	
λ_s (J/(kg °C))	53.00	1.95	0.60
C_f (W/(m °C))		4180	
C_s (W/(m °C))	460	341	108
e	0.0001	0.675	0.451

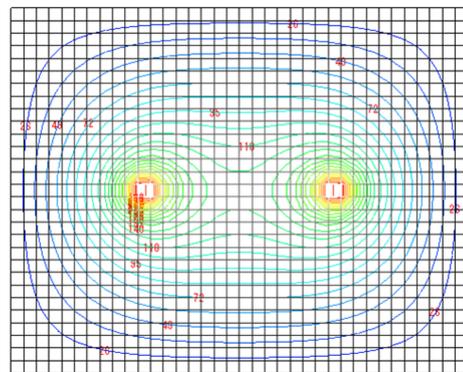


Fig. 7 Temperature distribution in the rock when temperature at waste becomes 300 °C.

by the thermal expansion of water. As the pressure becomes high, evaporation does not occur even if temperature is about 300 °C. It is, however, difficult to estimate the situation in the buffer material because the coarse mesh as shown in Fig. 7. Thus, the 1-D model is considered to estimate the detail situation in the buffer material in the following section.

4.2 1-D Detail Model

4.2.1 Model Description

As mentioned above, the buffer material was made with two elements from waste side to rock mass

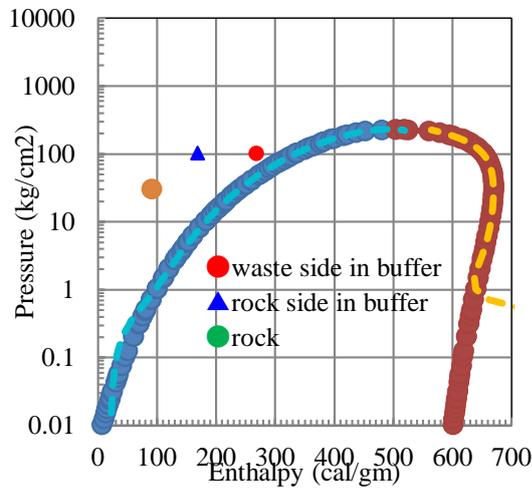


Fig. 8 Situation of phase at the different locations when temperature at waste becomes 300 °C

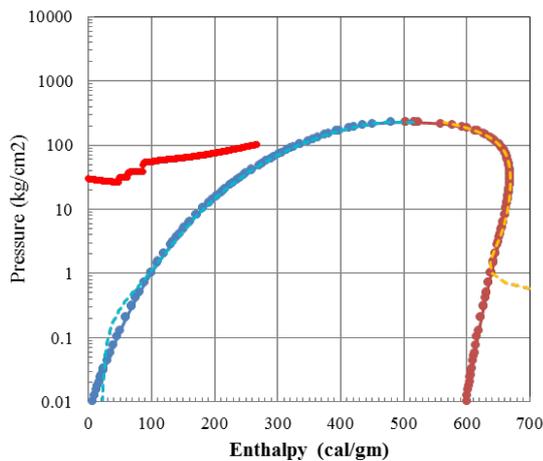


Fig.9 History of relation between pressure and enthalpy at the buffer material neighboring waste

side in 2-D model, the detail behavior in the buffer

material is difficult to discuss. Fig. 10 shows the schematic view of the 1-D model, which considers the previous concept of disposal with canister containing the waste package. The analysis region extends from the center of waste to the rock mass with the constant section of 1 m² and length of 25 m. The buffer material of which length is 0.72 m consists of 36 elements. The boundary conditions at the edge face of waste are the prescribed temperature as same as Fig. 6, no deformation for mechanical condition and no flow for hydraulic one. Temperature at the nodes in the waste region raises as shown in Fig. 6. The boundary conditions at the edge face of rock mass are the prescribed temperature of 15 °C, no deformation for mechanical condition and prescribed total head of 300 m. The other boundaries have no flow for thermal and hydraulic conditions and normal deformation fixed condition.

4.2.2 Analysis results of 1-D Model

Figs. 11-13 shows the histories of relation between pressure and enthalpy at the element neighboring the waste in the buffer material, the one at the center of the buffer material and the one neighboring rock in the buffer material. It is found that the buffer material neighboring the waste and rock enter into the two phase region as shown in Figs. 11 and 13. On the other hand, the part at the center of the buffer material is not at two phase region as shown in Fig. 12. This means that evaporation occurs at the both outer sides in the buffer material and evaporation does not occur at the inner parts in the buffer material.

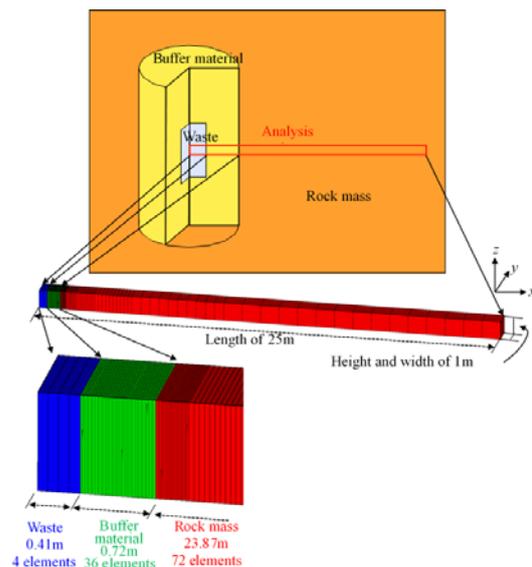


Fig. 10 Schematic view of the detail 1-D model

Fig. 14 shows the distribution of pressure in the buffer material. It is found that the pressure has the

largest value at the inner parts of the buffer material. The reason why evaporation does not occur at the inner parts is because the pressure of fluid at the inner parts becomes higher than that at the outer parts. Since temperature distributes mostly homogeneously in the buffer material, the high pressure may be caused from the result of fluid movement in the buffer material. This may be temporal situation and the situation of phase may change with time by depending on the boundary conditions and material properties. The verification of temporal situation change and validation of model are the remained tasks.

Moreover, the pressure becomes high at the boundary of liquid and two phase situation as shown in Figs. 12 and 13. The isothermal lines exit vertically at liquid region and become horizontally in two phase region as shown in Fig. 2. Therefore, the increase in temperature causes the increase in pressure close to the boundary between liquid and two phase region.

5. CONCLUSIONS

The disposal project of high level radioactive waste is very important for the countries having the nuclear plants. If the waste generates high heat, the effect of evaporation in the ground has to be considered for safe and stable disposal. The model to assess the effect of the evaporation of groundwater is developed in this study. The obtained conclusions are followings:

- 1) Evaporation process is dependent on temperature and pressure of fluid. It is found that the developed model has an ability to predict the complicated change in phase in the buffer material around the waste.
- 2) When temperature becomes large and the hydraulic conductivity is low, the fluid pressure may become very large because of the thermal expansion of fluid and difficulty of evaporation according to the circumstances.
- 3) While the results obtained in this study is very important, the verification of the phenomena and validation of the model are the remained subject.

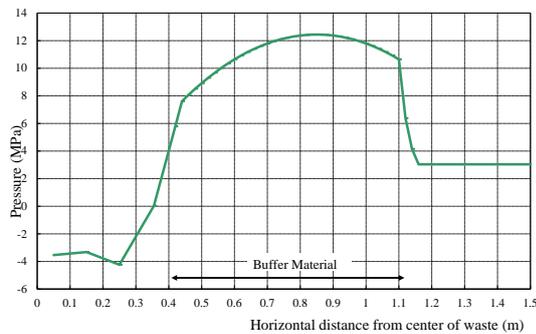


Fig. 14 Pressure distribution in the buffer material when temperature of the waste is 300 °C

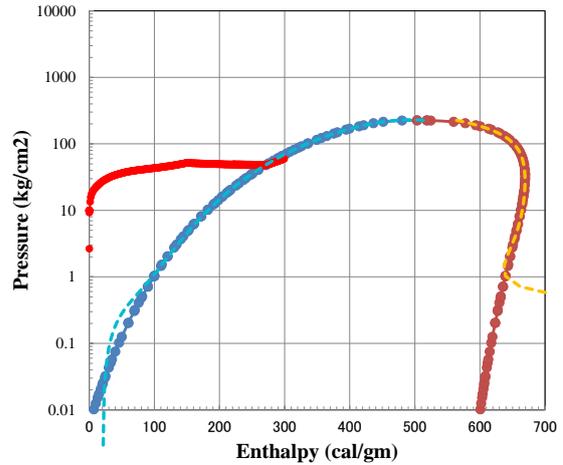


Fig. 11 History of relation between pressure and enthalpy at the element neighboring the waste in the buffer material

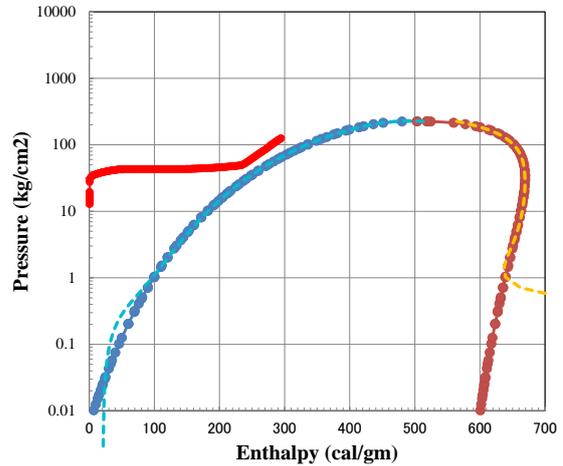


Fig. 12 History of relation between pressure and enthalpy at the element existing at the center of the buffer material

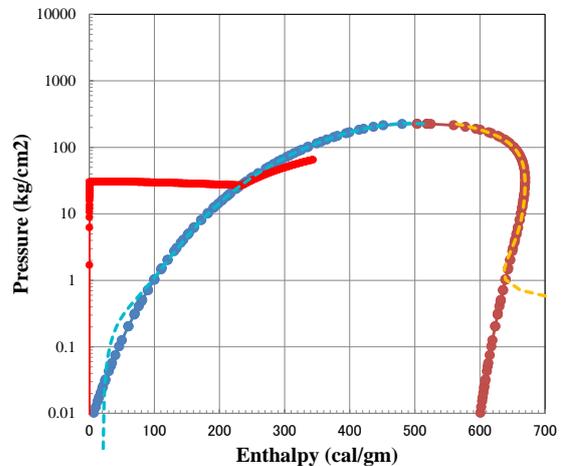


Fig. 13 History of relation between pressure and enthalpy at the element neighboring rock in the buffer material

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International Journal of GEOMATE, Sept, 2016, Vol. 11, Issue 25, pp.2403-2409.

MS No. 5275 received on June 11, 2015 and reviewed under GEOMATE publication policies.

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