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DEPRESSURIZATION ACCIDENT ANALYSIS OF MPBR BY PBR_SIM WITH CHEMICAL REACTION MODEL

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ABSTRACT

The simple model for natural circulation is implemented into PBR_SIM to provide air inlet velocity from the containment air space. For the friction and form loss only the pebble region is considered conservatively modeling laminar flow through a packed bed. For the chemical reaction model of PBR_SIM the oxidation rate is determined as the minimum value of three mechanisms estimated at each time step: oxygen mass flow rate entering the bottom of the reflector, oxidation rate by kinetics, and oxygen mass flow rate arriving at the graphite surface by diffusion. Oxygen mass flux arriving at the graphite surface by diffusion is estimated based on energy-mass analogy. Two types of exothermic chemical reaction are considered: ($C + zO_2 \rightarrow xCO + yCO_2$) and ($2CO + O_2 \rightarrow 2CO_2$). The heterogeneous and homogeneous chemical reaction rates by kinetics are determined by INEEL and Bruno correlations, respectively.

The instantaneous depressurization accident of MPBR is simulated using PBR_SIM with chemical model. The air inlet velocity is initially rapidly dropped within 10 hr and reaches a saturation value of about 1.5cm/s. The oxidation rate by the diffusion process becomes lower than that by the chemical kinetics above 600K. The maximum pebble bed temperatures without and with chemical reaction reach the peak values of 1560 and 1617 ^{O}C at 80 hr and 92 hr, respectively. As the averaged temperatures in the bottom reflector and the pebble bed regions increase with time, ($C+1/2O_2$->CO) reaction becomes dominant over ($C+O_2$->CO_2) reaction. Also, the CO generated by ($C+1/2O_2$->CO) reaction will be consumed by ($2CO+O_2$->$2CO_2$) reaction and the energy homogeneously generated by this CO depletion reaction becomes dominant over the heterogeneous reaction.

1. Natural Circulation Model of PBR_SIM

The simple model for natural circulation is implemented into PBR_SIM to provide air inlet velocity from the containment air space. For the friction and form loss only the pebble region is considered conservatively. For the friction and form loss in the pebble region the following Blake-Kozeny equation is used, modeling laminar flow through a packed bed:

$$\Delta p_f = H \times (150 / d_p^2)(1-e)^2 / e^3 m_{hot} v_{hot}$$

where H, d_p, e : height of pebble bed, diameter of a pebble bed, porosity

m_{hot}, v_{hot} : viscosity and velocity of gas mixture at averaged temperature in the pebble bed region

This correlation is used instead of the more complicated correlation because of its no requirement of iteration. The buoyancy driving force is expressed as follows:

$$\Delta p_d = (r_{cold} - r_{hoy}) g H$$

where r_{cold}, r_{hot} : averaged gas densities in the cold and hot sides

The average air velocity is calculated balancing the above two pressure drop:

$$v_{av} = C(r_{cold} - r_{hot}) / m_{av}$$

$$where\ C = g / [(150(1-e)^2 / (d_p^2 e^3)]$$

It can be noted that the average gas velocity only depends on the ratio of the density difference to the gas viscosity, which increase with an increase in the hot side temperature given the cold side temperature.

In case of the rupture of stand pipe and hot gas duct, the cold temperature in the air gap region is conservatively determined, taking arithmetical average between the average temperature in the top reflector and the containment sink temperature, 100 °C. It means that the gas mixture with the top reflector temperature is exiting the ruptured stand pipe and will be cooled down up to the containment sink temperature before it reaches the bottom of the air gap region. In case of rupture of hot and cold gas ducts, the cold temperature in the annular region of the reactor vessel is conservatively determined, taking arithmetical average between the top reflector temperature and the reactor vessel temperature. Also, it means that the gas mixture with the top reflector temperature is entering the annular region and will be cooled down up to the reactor vessel temperature.

It is assumed that only air will enter the broken ducts and all the oxygen in the air will be consumed in the bottom reflector. Also, no heat removal by convection of gas mixture and endothermic reaction of ($2C,O_2$) will be credited. Therefore, the results produced by PBR_SIM are expected to be very conservative.

The total air flow rate entering the reactor vessel through the hot gas duct is estimated as

$$W_{airin} = (rv)_{airin} A_{fpebble}$$

where $v_{airin} = v_{av} \times (r_{av} / r_{air,in})$: air inlet velocity(m/s), where air inlet density is determined at 20C

$A_{fpebble}(m^2)$: flow area in the pebble bed region estimated with the assumption that its permeability is the same as its porosity

Note that the averaged velocity of the gas mixture does not depend on the height of the pebble bed but totally depends on the ratio of the density difference to the viscosity. Both of the ratios of the density difference and the viscosity increase with the averaged pebble bed temperature. While the inlet velocity scaled at 20°C decreases for 400K in the cold side, those for both of 500K and 600K in the cold side increase at the lower averaged pebble bed temperature but decrease at the higher temperature as shown in Fig.1. Also, the air velocity is highly and mildly sensitive to the temperatures in the cold side and the hot side, respectively.

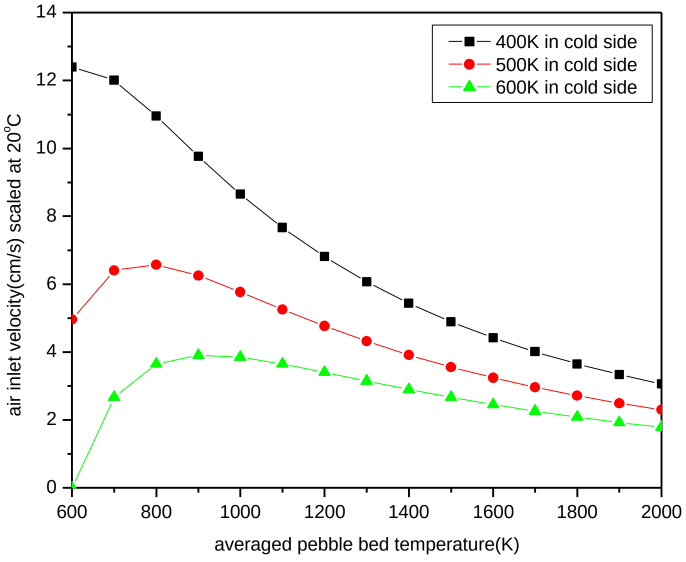

Fig.1. Air inlet velocity scaled at 20 °C

2. Chemical Reaction Model of PBR_SIM

The following heterogeneous reactions between the graphite and gas are considered:

$C + zO_2 \rightarrow xCO + yCO_2$:

$C + O_2 \rightarrow CO_2$: $\Delta H^{C\_O_2}_{CO_2} = 394$ kJ/mol (exothermic)

$C + 1/2O_2 \rightarrow CO$: $\Delta H^{C\_O_2}_{CO} = 111$ kJ/mol (exothermic)

$C + CO_2 \rightarrow 2CO$: $\Delta H^{C\_CO_2}_{CO} = -172$ kJ/mol (endothermic)

$C + H_2O \rightarrow CO + H_2$: $\Delta H^{C\_H_2O}_{CO} = -118.5$ kJ/mol (endothermic)

The homogeneous reaction in the gas mixture considered is as follows:

2CO + O_2 → 2CO_2 : $\Delta H_{CO_2}^{CO\_O_2} = 565.98$ kJ/mol (exothermic)

Here, two exothermic chemical reactions (C, O2) and (CO, O2) are considered.

The oxidation rate is determined as the minimum value of three ones estimated at each time step: oxygen mass flow rate entering the bottom of the reflector, oxidation rate by kinetics, and oxygen mass flow rate arriving at the graphite surface by diffusion.

Oxygen mass flux arriving at the graphite surface by diffusion is estimated based on energy-mass analogy. According to the analogy the Sherwood number is defined as

$$Sh = k_m D\ / D_{ab} = Nu(Sc/\mathrm{Pr})^{1/3}$$

where k_m, D, D_{ab}: mass transfer coefficient, characteristic diameter, diffusion coefficient between mixture and CO_2.

$$D_{ab} = (0.00143T^{1.75})/\{pM_{ab}^{1/2}[\Sigma_{va}^{1/3} + \Sigma_{vb}^{1/3}]^2\}$$

$$M_{ab} = 2/(1/M_a + 1/M_b)$$

Σ_{va}, Σ_{vb}: diffusion volume (19.7 for air and 26.9 for CO_2)

p, T: temperature and pressure in the gas mixture

For laminar flow in the pipe the following asymptotical Nu for constant wall temperature is used:

Nu=3.657

The oxygen mass flux arriving at the graphite surface, G_d, is estimated as

$$G_d = (M_c/M_{O_2})r_{O_2}k_m$$

where M_c, M_{O_2}, r_{O_2} : molecular weights of C and O_2, and density of O_2

The oxygen mass flow rate arriving at the total interfacial surface becomes

$$W_d = A_i G_d$$

where A_i : interface area between the graphite wall and the gas mixture

The volumetric mass flow rate is estimated as

$$\Gamma_d^{C\_CO_2} = z * G_d A_i / V$$

where V: volume of bottom reflector

Here, z is defined in the (C, O_2) chemical reaction of (C + zO_2 → xCO + yCO_2).

The chemical reaction rate by kinetics is described as

$$r_{C\_O_2}(kg/m^2s) = K_1 \exp(-E_1/T)(p_{O_2}/20900)$$

where K_1, E_1: 0.2475 and 5710 for T<1273K, and 0.0156 and 2260 for 2073K>T>1273K, in which are determined by INEEL correlation

R: universal gas law constant=8314J/(kg-mole*K)=8.314*10^{-3}kJ/g-moleK

p_{O_2} : oxygen partial pressure whose value in the fresh air is 20900Pa.

The mass depletion rate and production rates of O_2, CO, and CO_2 per unit graphite volume (kg/m^{3}s) are estimated as

$$\Gamma_{O_2}^{C\_O_2} = -z r_{C\_O_2}(M_{O_2}/M_C)*(A_i/V_g),$$

The depletion rate of oxygen is controlled by chemical kinetics, diffusion process, and the supply of oxygen:

$$\Gamma_{O_2}^{C\_O_2} = -\min(r_{C\_O_2} C_{mol} M_{O_2}, W_{in} f_{O_2}/V_g, \Gamma_d^{C\_O_2})$$

Then, the new mass production rates of CO_2 and CO are estimated with the above depletion rate of oxygen:

$$\Gamma_{CO_2}^{C\_O_2} = -\Gamma_{O_2}^{C\_O_2}(y/z)(M_{CO}/M_{O_2})$$

$$\Gamma_{CO}^{C\_O_2} = -\Gamma_{O_2}^{C\_O_2}(x/z)(M_{CO_2}/M_{O_2})$$

Here, the production ratio of CO to CO_2 (A=x/y) in the chemical reaction of (C, O2) is correlated as follows:

$$A = 7943\exp(-78.3/(RT)) = 7943\exp(-9417.8/T)$$

Then, the following relations can be obtained:

z=0.5(A+2)/(A+1), x=A/(A+1), y=1/(A+1)

The fraction of CO produced rapidly increases with the graphite temperature around 1050K as shown in Fig.2.

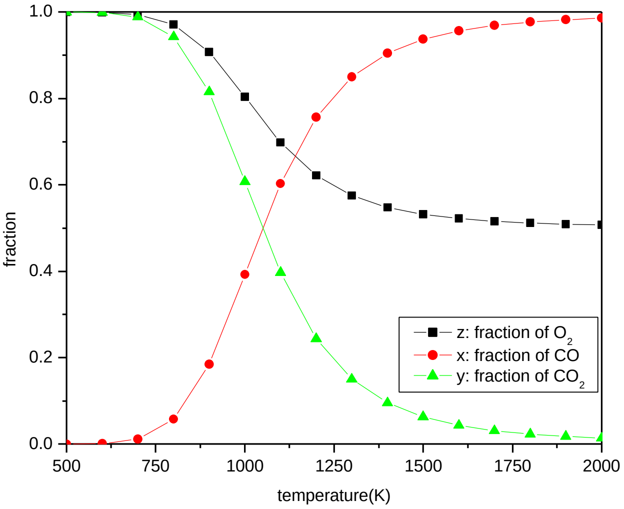

Fig. 2. Chemical reaction: C+zO2->xCO+yCO2

With the fraction of O_2, z, the O_2 dissipation rates with the graphite temperature is estimated by the chemical kinetics and the diffusion process. In both cases the oxygen pressure in the air is used as that in the bottom reflector and its diameter is 2cm. As shown in Fig.3, the oxidation rate by the diffusion process becomes lower than that by the chemical kinetics around 600K. The oxidation rate by the diffusion process is insensitive to the graphite temperature because of the reduction of z with the graphite temperature.

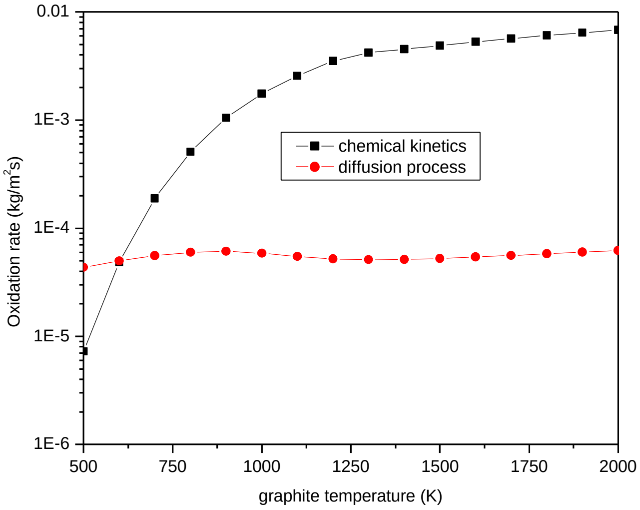

Fig. 3: Oxidation rate vs. graphite temperature for kinetics and diffusion process

The reaction rate of the CO combustion is taken from Bruno:

$$dC_{CO}/dt = -r_{CO-O_2} C_{CO} C_{O_2}^{1/2} C_{H_2O}^{1/2}$$

where C_i: mole concentration(mole/m^3) of i-component gas estimated as

$$C_i = \rho_i / M_i = \rho w_i / M_i$$

$w_i = \rho_i / \rho$: mass fraction of i-component gas

ρ: mixture density

The mole concentration of steam is expressed as

$$C_{H_20} = 0.0054C .$$

where C: mixture concentration

It is known that gas phase oxidation of CO requires OH radicals which are produced at the graphite wall from H_2O and attack the CO molecules. As a result, the presence of water increases the catalytic oxidation rate of CO. However, as H_2O itself is consumed by chemical reaction between it and graphite, the reaction rate of the CO combustion will be largely reduced due to a decrease in the concentration of H_2O.

Here, the reaction rate, r_{CO-O_2}, is described as

$$r_{CO-O_2} = 1.3*10^{11}\exp(-15155.2/T).$$

The dissipation rate of CO is expressed as

$$\Gamma_{CO}^{CO-O_2} = (dC_{CO}/dt)M_{CO}$$
$$\Gamma_{O_2}^{CO-O_2} = 0.5\Gamma_{CO}^{CO-O_2}(M_{O_2}/M_{CO})$$
$$\Gamma_{CO_2}^{CO-O_2} = -\Gamma_{CO}^{CO-O_2}(M_{CO_2}/M_{CO})$$

The total dissipation rates and the production rates of O_2, CO, and CO_2 per unit graphite volume become

$$\Gamma_{O_2} = \Gamma_{O_2}^{C-O_2} + \Gamma_{O_2}^{CO-O_2}$$
$$\Gamma_{CO_2} = \Gamma_{CO_2}^{C-O_2} + \Gamma_{CO_2}^{CO-O_2}$$
$$\Gamma_{CO} = \Gamma_{CO}^{C-O_2} + \Gamma_{CO}^{CO-O_2}$$

The whole graphite region is needed to be divided into two regions: bottom reflector region and pebble bed region. The general mass balance of each gas species in the bottom reflector and the pebble bed region becomes

$$(M_{gi}^{n+1} - M_{gi}^{n})/\Delta t = W_{giin} - W_{giout} + \Gamma_{gi}V_b$$
$$-> r_{gi}^{n+1} = r_{gi}^{n} + \Delta t(W_{giin} - W_{giout})/V_{gi} + \Delta t\Gamma_{gi}V_b/V_{gi}$$

where subscript, gi: i-component gas species

M_{gi}, r_{gi} : mass and density of i-component gas species in each region

W_{giin}, W_{giout}: mass flow rates of i-component gas species at the inlet and outlet of each region

Γ_{gi} : mass generation rate of i-component gas species per graphite volume in each region

V_{gi} : gas volume in each region

The concentration of the i-component gas species is obtained as

$$C_{gi} = r_{gi}/M_i$$

The density and concentration of the gas mixture are also obtained as

$$r = \sum r_{gi}, C = \sum C_{gi}$$

For the continuity of oxygen with the assumption that the velocity of each i-component species is the same as the mixture velocity, we have

$$r_{O_2}^{n+1} = r_{O_2}^{n} + \Delta t(W_{O_2in} - W_{O_2out})/V_{gi} + \Delta t\Gamma_{O_2}$$

where $W_{O_2in} = W_{airin} \times f_{O_2}$ in the bottom reflector region

$$W_{O_2out} = r_{O_2} v_{out} A_f$$

For the continuity of CO$_2$

$$r_{CO_2}^{n+1} = r_{CO_2}^{n} + \Delta t(W_{CO_2in} - W_{CO_2out})/V_{gi} + \Delta t \Gamma_{CO_2} V_b / V_{gi}$$

where $W_{CO_2in} = W_{airin} \times f_{CO_2}$ in the bottom reflector region

$$W_{CO_2out} = r_{CO_2} v_{out} A_f$$

For the continuity of CO

$$r_{CO}^{n+1} = r_{CO}^{n} + \Delta t(W_{COin} - W_{COout})/V_{gi} + \Delta t \Gamma_{CO} V_b / V_{gi}$$

where $W_{COin} = W_{airin} \times f_{CO}$ in the bottom reflector region

$$W_{COout} = r_{CO} v_{out} A_f$$

The pressure of an i-gas species is estimated as

$$p_i = R\, T(r_i / M_i)$$

where T: volume-averaged graphite temperature in each region

It is assumed that the pressure of mixture in the reactor vessel is the same as the atmospheric pressure:

$$p_{atm} = p_{N_2} + p_{O_2} + p_{CO_2} + p_{CO} = RT\sum(r_i / M_i)$$

where R: universal gas law constant=8314 J/(kg-mole*K)

Then, the partial pressure and density of nitrogen are estimated as

$$p_{N_2} = p_{atm} - (p_{O_2} + p_{CO_2} + p_{CO}) = p_{atm} - RT[(r/M)_{O_2} + (r/M)_{CO} + (r/M)_{CO_2}]$$

$$r_{N_2} = (p_{N_2} M_{N_2})/(RT)$$

As the continuity of mixture is expressed as

$$r^{n+1} = r^{n} + \Delta t(W_{in} - W_{out})/V_{gi} + \Delta t \sum \Gamma_{gi} V_b / V_{gi},$$

we have the velocity at the top of the bottom reflector as

$$v_{out} = \{W_{airin} + V_{gi}[(r^{n} - r^{n+1})/\Delta t + \sum \Gamma_{gi} V_b]\}/(r_{out} A_f)$$

3. Simulation of Rupture of Coaxial Ducts by PBR_SIM with chemical model

The instantaneous depressurization accident, in which shutdown and complete depressurization at the start of accident take place, is simulated using PBR_SIM with chemical model. The averaged pebble bed temperature and averaged annular passage temperature are initially rapidly increased as shown in Fig. 4.

As a result, the air inlet velocity is initially rapidly dropped within 10 hr and reaches a saturation value of about 1.5cm/s as shown in Fig. 5.

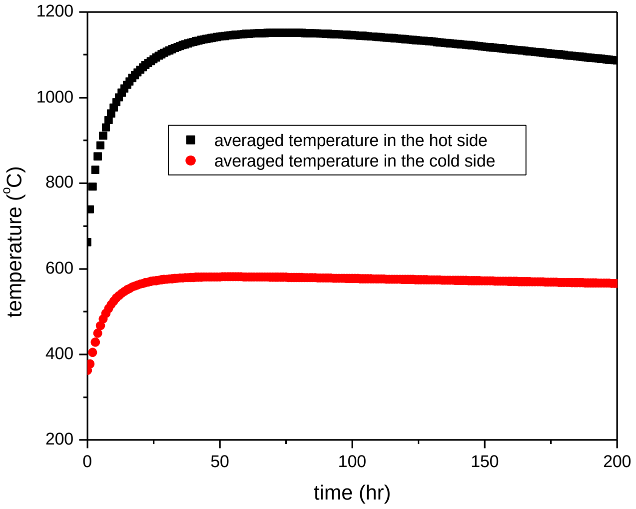

Fig. 4. Averaged temperature trend in the cold and hot sides

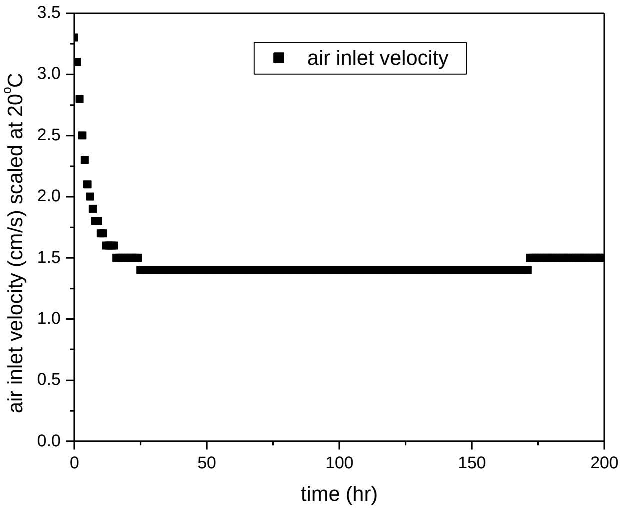

Fig. 5. Air inlet velocity scaled at 20 °C

As the air ingress starts, the concentration of oxygen in the bottom reflector rapidly increases and, as a result, the chemical generation rates in the bottom reflector and the pebble bed regions rapidly increase as shown in Fig. 6. Then, they reach the saturation values in the same way as the air flow rate entering the bottom reflector does. The chemical energy generation rate in the bottom reflector is much higher than that in the pebble bed region. Up to 200hr the decay heat is dominant over the total chemical generation rate.

The total masses of oxygen depleted in the bottom reflector and the pebble bed region are almost linearly increased with time. With the confinement volume of 3,000m^3, all oxygen will be depleted within 6hrs.

Three cases are investigated: the original model for graphite oxidation rates, INEEL correlation for graphite oxidation rate with the axial conduction-radiation energy transfer, INEEL correlation for graphite oxidation rate without the axial conduction-radiation energy transfer. INEEL correlation gives the highest oxygen consumption rate in the bottom reflector. Therefore, it produces the highest temperature increase in the bottom reflector as shown in Fig. 7.

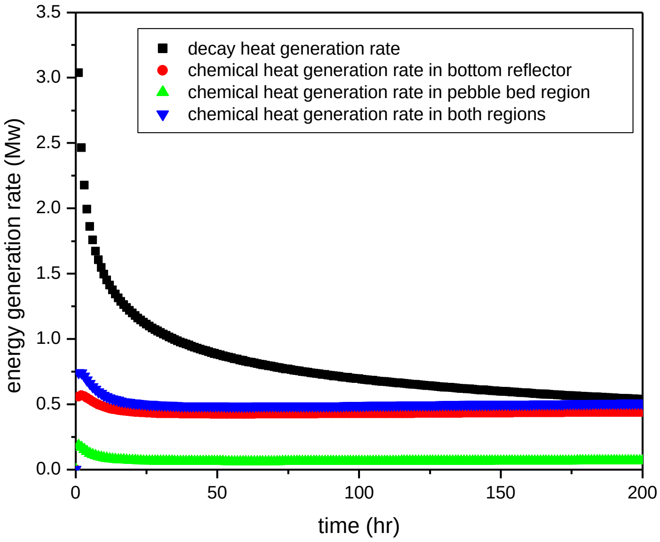

Fig. 6. Comparison between decay heat and chemical heat generation rates

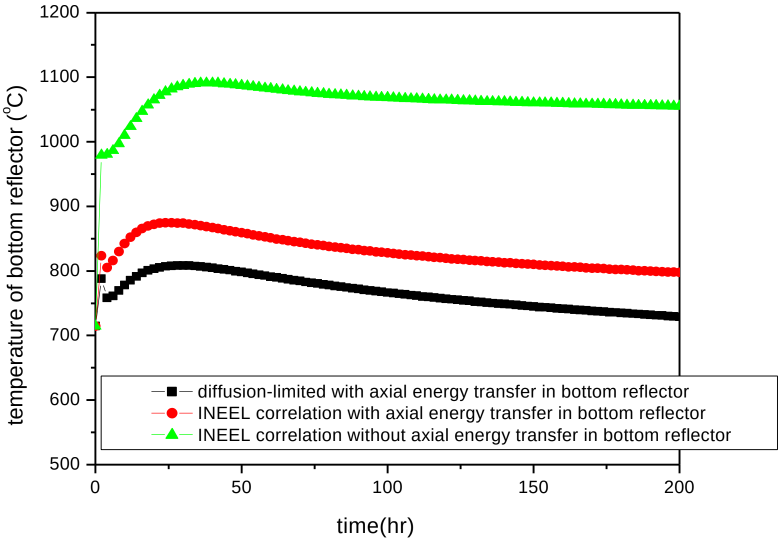

Fig. 7. Comparison of temperature trend of bottom reflector with INEEL correlation and diffusion-limited correlation

However, the model dealing with the axial energy transfer of conduction and radiation in the bottom reflector region plays a more important role in the temperature in the bottom reflector region than the model related to the graphite oxidation. However, in the pebble bed region the trend becomes reverse: the maximum pebble bed temperature with the INEEL correlation is a little lower than that with the diffusion-limited model as shown in Fig.8 because the INEEL model drives more oxygen in the bottom reflector to be consumed and less one to be available for graphite oxidation in the pebble bed region. Also, the effect of the inclusion of the axial model in the bottom reflector on the maximum pebble bed temperature is very small because most of oxygen is consumed in the bottom reflector. In the pebble bed region the mole fraction of oxygen is very small as shown in Fig. 9.

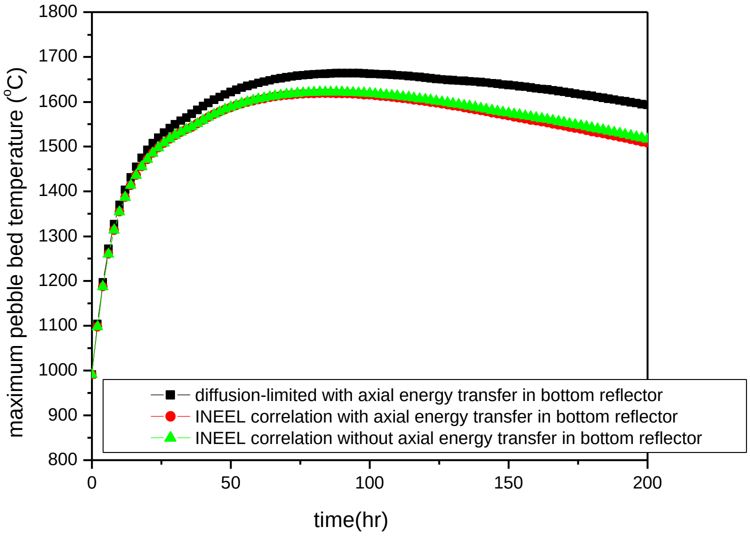

Fig. 8. Comparison of trends of maximum pebble bed temperature

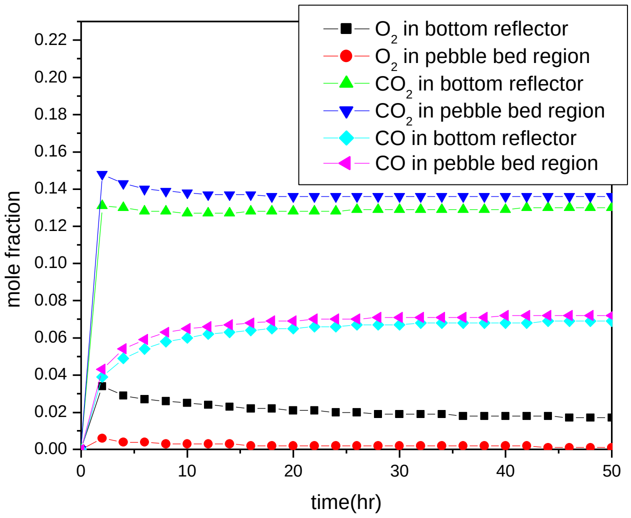

Fig.9. Averaged mole fraction in bottom reflector and pebble bed region

Conclusions

The simple model for natural circulation and chemical reaction model are implemented into PBR_SIM to analyze the depressurization accident of MPBR. The air inlet velocity is initially rapidly dropped within 10 hr and reaches a saturation value of about 1.5cm/s. The diffusion process above the graphite temperature of 600K limits the oxidation rate. The maximum pebble bed temperatures without and with chemical reaction reach the peak values of 1560 and 1617 ^{O}C at 80 hr and 92 hr, respectively. As the averaged temperatures in the bottom reflector and the pebble bed regions increase with time, ($C+1/2O_2 \rightarrow CO$) reaction becomes dominant over ($C+O_2 \rightarrow CO_2$) reaction. Also, the CO generated by ($C+1/2O_2 \rightarrow CO$) reaction will be consumed by ($2CO+O_2 \rightarrow 2CO_2$) reaction and the energy homogeneously generated by this CO depletion reaction becomes dominant over the heterogeneous reaction.

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