Comparing the formation and propagation features of subcritical and supercritical thermal detonation waves

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Abstract. During a severe accident in a nuclear reactor, an ex-vessel steam explosion may occur when the molten core come into contact with the liquid coolant, the crucial factor in the fuel-coolant interaction is the fragmentation of melt into small droplets, which rapidly increase the heat transfer to the coolant, and could lead to a steam explosion and formation of a pressure wave with a disastrous consequence for the surrounding components. In this research a numerical simulation of a steam explosion was performed using the VAPEX-D code which is being developed at the Department of NPP in “Moscow Power Engineering Institute” for the simulation of fuel-coolant interactions. Using the microinteractions concept, the propagation of thermal detonation waves was studied, and the characteristics of subcritical and supercritical waves were compared. A sharp increase in pressure is noted during the transition from subcritical mode to supercritical mode of propagation. A parametric study was performed where the volume fraction of corium was varied to determine the critical value at which the thermal detonation wave decayed. The study shows that increasing the melt volume fraction, will increase the maximum pressure and the velocity of the thermal detonation wave. While varying the initial void fraction showed that the thermal detonation wave can propagate in a very low melt volume fraction.

1. Introduction

During the development of a severe accident with core melt in a nuclear power plant, the molten core (corium) may come into contact with the liquid coolant (water or sodium). At certain conditions the corium-coolant system is capable of explosive interaction with increasing pressure up to hundreds and even thousands of bars, which can endanger the containment. This phenomenon is known as steam explosion, and is being actively studied in many scientific centers of nuclear energy. At present, it is generally accepted that the development of a steam explosion goes through the following stages [1]:

1. Preliminary mixing of corium-coolant and formation of a coarse mixture (melt drops dispersed in coolant and surrounded by a film of vapor);
2. Triggering event;
3. Propagation of thermal detonation wave, which cause fragmentation of the large melt drops, that enhance thermal energy transfer from melt to the coolant;
4. The expansion of the steam explosion products in the surrounding medium.

In this paper, we analyzed the third stage of the steam explosion (the propagation of thermal detonation wave). The basic theoretical background of the fuel-coolant explosions is presented in [2]. The key phenomena that determine the parameters of the steam explosion is the fragmentation of large (of the order of several millimeters) melt drops into small fragments (tens of microns), which leads to a sharp increase of heat transfer from the melt to the surrounding coolant. In this study we compared the characteristics of the propagation of subcritical and supercritical thermal detonation waves using the code VAPEX, which is developed at the Department of NPP of National Research University "Moscow Power Engineering Institute" [3-5]. This work is a continuation of the study [6], in which only the behavior of the subcritical thermal detonation wave was analyzed.

2. Description of the thermal detonation model used in the VAPEX code

The model of thermal detonation in the VAPEX code is based on the concept of “microinteractions” [7, 8]. This approach assumes that the small melt fragments formed during the fragmentation of the large melt drops, transfer their energy and momentum not to the entire coolant, but only to a small part located near these fragments. The concept is based on the fact, that the time to reach thermal equilibrium in the coolant (determined by the coolant thermal conductivity) is significantly longer than the time of heating the coolant by the melt fragments in the fragmentation zone along the detonation wave (determined by the propagation velocity of the detonation wave through the fragmentation zone). The remaining coolant, which is not involved in the interaction with the melt, still affects the dynamics of the process development. Thus, introducing the concept of microinteractions zone leads to thermal nonequilibrium in the system, where one part of the coolant directly adjacent to the fragments is involved in the development of thermal detonation, and the other part surrounding the explosive interaction zone, influences the process by hydrodynamic interaction with the interaction zone.

To describe the multiphase dynamics, a multi-fluid approach is used [9]. Four fluids are considered: large (initial) drops of melt (f-fluid); “far” coolant (not in direct contact with the melt fragments, l-fluid); the field of microinteractions (coolant in the direct vicinity of the fragments, m-fluid); small fragments of melt droplets formed after fragmentation (db-fluid). It is assumed that the m-fluid is vapor and is in thermal and velocity equilibrium with the db-fluid, i.e. the resulting fragments of the melt instantly transfer heat to the surrounded coolant, leading to evaporate it. Thus, the governing equations determining the propagation of the thermal detonation wave includes: four continuity equations, three momentum conservation equations, and three energy conservation equations. The exchange of energy, momentum and mass between phases is considered. Since the melt fragments are surrounded by the m-fluid, there is no exchange of momentum and energy between the fragments and the coolant in the l-fluid, as well as large melt drops of the f-fluid. It is also assumed that the large drops and small fragments of the melt have a constant uniform density.

3. Numerical simulation of thermal detonation wave propagation

We will consider a half-space domain bounded on the left side by a solid wall, and filled with a steam-water mixture and coarse melt drops. Due to the high propagation velocity of the thermal detonation wave, the gravity effect is not taken into account. To initiate the thermal detonation, a high-pressure region (trigger zone) of 3 cm long is set near to the solid wall. Because of the pressure drop at the boundary, the medium begins to move, which initiates the fragmentation of melt drops and the formation of a thermal detonation wave.

The calculations were performed corresponding to the conditions of an ex-vessel steam explosion with the following system parameters: initial pressure of 0.4 MPa, the steam-water mixture is saturated. We studied the reactor core melt, consisting of 80% (wt.) of uranium dioxide and 20% (wt.) of zirconium dioxide. Thermophysical properties of corium: density 7960 kg/m³, heat capacity 565 J/(kg·K), surface tension coefficient 0.45 N/m. We used typical values as: the initial temperature of the corium 2800 K and the diameter of the corium drops 5 mm.
4. Propagation of a subcritical detonation wave
The first case we considered is when the initial void fraction equal to 0.5. A series of calculations was carried out with the aim of revealing the volume fraction of the melt below which a steady state thermal detonation wave does not exist.

At sufficiently high melt volume fractions, and after a certain transition process, a steady state propagation of the thermal detonation wave is observed. The characteristics of this wave is not depended on the pressure in the trigger zone (which varied in the range of 10-100 bar). Figure 1 shows a typical picture of the development of a thermal detonation wave, pressure profiles are shown at successive times (0.1 ms, 0.5 ms, 1 ms, 1.5 ms, 2 ms, 2.5 ms, 3 ms, 3.5 ms, 4 ms, 5 ms, 6 ms, 7 ms, 8 ms, 9 ms, 10 ms, 11 ms, 12 ms, 12.5 ms) for the case when the melt volume fraction is 0.008. It can be seen from the figure 1 that approximately after 4 ms, a steady state pressure wave is generated, with an amplitude of 129 bar, and propagation velocity of 207 m/s. The length to reach the steady state is approximately 0.8 m. It should be noted that this length and its corresponding time depend on the pressure in the trigger region. The closer to the pressure in the steady state detonation wave, the smaller the length and the time needed to reach the steady state.

Figures 2 and 3 show the velocity profiles of the steam and water at the same moments of time as in figure 1. By the time of reaching the steady state, the approximate velocities of steam and water are 120 m/s and 85 m/s, respectively. From figure 4 it follows that not all of the melt is fragmented in the thermal detonation wave. Approximately 25% remain unfragmented.

5. Extinction of the thermal detonation wave at small volume fractions of fuel
With decreasing the melt volume fraction, the thermal detonation wave does not reach the steady state, but gradual extinction occurs, which is illustrated in figure 5. The melt volume fraction in this
calculation is equal to 0.006, and the void fraction is equal to 0.5. Figures 6-8 show the profiles of the volume fractions of the mixture components (steam-water-melt) at various moments of time (1 ms, 2 ms, 3 ms, 5 ms, 7 ms, 8 ms, 9 ms, 10 ms, 11 ms), while figures 9, 10 show the profiles of the velocity of steam and water.

Figure 5. The development of the pressure profile.

Figure 6. The development of the steam volume fraction profile.

Figure 7. The development of the water volume fraction profile.

Figure 8. The development of the melt volume fraction profile.
6. Formation and propagation of a supercritical detonation wave
With increasing the melt volume fraction, supercritical thermal detonation is observed. The features of this process are shown in figures 11-15. Figure 11 show the profiles of pressure at various moments of time (1 ms, 2 ms, 3 ms, 4 ms, 5 ms, 6 ms, 7 ms, 8 ms) for an initial fuel fraction of 0.021.

Figures 12, 13 show the velocity profiles of the steam and water. By the time of reaching the steady state, the steam velocity is approximately 450 m/s, and the water velocity is equal to 340 m/s. These velocities significantly exceed the velocities in the case of subcritical detonation. For the steam, the difference is 375%, for the water – 400%.
From figure 14 it follows that, in contrast to the case of subcritical thermal detonation, in which approximately 25% of the melt remains not fragmented, in the case of supercritical detonation, the entire melt is fragmented.
Figures 16, 17 illustrate that in the supercritical region the steam temperature changes quite strongly, reaching 1700 K, while the initial temperature was 420 K, while the water practically does not heat up (by the time of reaching the steady state, the water temperature changes compared to the initial is 20 K). The supercritical region is still divided into two regions: steam-like region and water-like region.

7. Summary results of the parametric calculations of the thermal detonation
Parametric calculations were carried out, in which the volume fraction of corium was varied to determine the critical volume fraction value at which the thermal detonation wave was attenuated. The calculation results are presented in table 1, which presents the characteristics of the thermal detonation wave at various melt volume fractions.

From table 1 it follows that with increasing the melt volume fraction, the maximum pressure and the velocity of the thermal detonation wave also increase. A sharp increase in pressure (by an order of magnitude) is noted during the transition of a thermal detonation wave from a subcritical mode to a supercritical mode of propagation (with a melt volume fraction equal to 0.019).

| Melt volume fraction | Maximum pressure, bar | Thermal detonation wave velocity, m/s |
|----------------------|------------------------|-------------------------------------|
| 0.006                | Thermal detonation wave extinction |
| 0.007                | 48                     | 133                                 |
| 0.008                | 86                     | 176                                 |
| 0.009                | 129                    | 207                                 |
| 0.0095               | 152                    | 223                                 |
| 0.01                 | 176                    | 234.4                               |
| 0.019                | 2100                   | 698                                 |
| 0.02                 | 2190                   | 709                                 |
| 0.021                | 2265                   | 709                                 |

In order to study the effect of void fraction on the development of the thermal detonation wave, we performed calculations at lower values of this parameter. The results showed that the region of existence of a stable thermal detonation wave is extended, in particular, when the melt volume fraction is equal to 0.005, and the void fraction is equal to 0.5, the thermal detonation wave decays, while in the case of void fraction equal to 0.25, a stable thermal detonation wave is observed. However, with a small decrease in melt volume fraction to 0.004, the thermal detonation wave decays. Thus, when the void fraction is 0.25, the boundary value of the volume fraction of the melt at which there is a thermal detonation wave is 0.0045.

8. Conclusion
1. Using the VAPEX-D code, a numerical simulation of an ex-vessel steam explosion was performed to study the development of a thermal detonation wave in the system of corium-steam-water, using the model of microinteractions. Depending on the melt volume fraction, both the steady-state propagation of the thermal detonation wave, and the wave extinction were obtained.
2. A sharp increase in pressure (by an order of magnitude) was obtained during the transition of a thermal detonation wave from a subcritical mode to a supercritical propagation mode (with a melt volume fraction of 0.019).
3. With a decrease in the initial void fraction, the minimum melt volume fraction at which a thermal detonation wave occurs also decreases. The calculation results indicate that a thermal detonation wave can develop in very poor mixtures (melt volume fractions equal to 0.005-
0.01). Despite the fact that the resulted pressures are relatively small (200-400 bar), however, that can initiate a strong steam explosion in areas where the volume fraction of the melt is much higher (of the order of 0.1), accordingly, much larger dynamic loads on the NPP equipment is developed.

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