NUMERICAL ANALYSIS OF VAPOR EXPLOSION IN THE SYSTEM "CORIUM-WATER"

O.I. Melikhov, V.I. Melikhov and A.V. Sokolin

Electrogorsk Research and Engineering Centre on NPPs Safety

Bezymyannaya 6, Electrogorsk, 142530, Russia

oleg.melikhov@erec.ru, vladimir.melikhov@erec.ru,
alex.sokolin@erec.ru

ABSTRACT

The thermal detonation taking into account the microinteraction processes model has been applied to study thermal detonation wave escalation and propagation in the corium-water mixture. Transient escalation stage and subsequent steady-state propagation stage of the thermal detonation have been calculated. The essential decrease of the escalation length in comparison with the previous results calculated without microinteraction concept has been obtained.

1   INTRODUCTION

A thermal detonation as a way of realization of large-scale fuel-coolant energetic interaction (vapor explosion) was first proposed in [2]. They used analogy between thermal system (mixture of hot liquid fuel droplets and cold volatile liquid) and chemical system (combustible gases) to develop thermal detonation theory. The further works ([1], [7], [10], [14], [15] and [16]) developed steady-state models of thermal detonation. They carried out detailed investigations of the effect of fragmentation, heat transfer, losses. However, applicability of these works is restricted to steady-state, fully developed detonations.

Another direction of the thermal detonations studies is a transient modeling. The first transient model of thermal detonation has been developed in [5]. Subsequent works ([3], [4], [6], [8], [9], [11], [13] and [17]) essentially developed thermal detonation model. Different systems, geometries and fragmentation mechanisms were considered. Thermal detonation escalation in the system "corium-water" up to achievement of the steady-state propagation has been numerically analyzed in [12].

In the present work the microinteraction concept proposed by Theofanous with co-authors [6] has been introduced in the model of thermal detonation and the problem concerning approach of the steady-state stage has been considered. The essential decrease of the transient distance of the detonation wave in comparison with the results of the previous work [12] was obtained.

2   MATHEMATICAL MODEL

We have considered transient one-dimensional planar propagation of the thermal detonation wave in the system "corium-water". The initial mixture ahead of the detonation front is assumed to consist of fuel (melt) drops and coolant. Behind the detonation front the drops are fragmented and microinteraction concept is used for description of fragmentation process. In accordance with this concept initially only a small quantity of coolant around each coarsely premixed melt mass "sees" the fragmenting debris coming off it. The rest of the coolant simply does not participate in the ensuing thermal interaction, but it does participate in the wave dynamics process.

So, there are four phases under consideration: namely, "microinteraction" fluid (m-fluid), coolant, fuel drops and fuel debris. They will be referred to as m-fluid, liquid, fuel and debris respectively. Each phase is represented by one flow field with its own local concentration and temperature. The debris is assumed to be part of the m-fluid in thermal and hydrodynamic equilibrium. Thus we have four continuity equations, there momentum equations, and three energy equations.

Continuity Equations

m - Fluid:

$$\frac{\partial \alpha_m \rho_m}{\partial t} + \frac{\partial (\alpha_m \rho_m u_m)}{\partial x} = E + J \tag{1}$$

Liquid:

$$\frac{\partial \alpha_l \rho_l}{\partial t} + \frac{\partial (\alpha_l \rho_l u_l)}{\partial x} = -E - J \tag{2}$$

Fuel:

$$\frac{\partial \alpha_f \rho_f}{\partial t} + \frac{\partial (\alpha_f \rho_f u_f)}{\partial x} = -F_r \tag{3}$$

Debris:

$$\frac{\partial \alpha_{db} \rho_{db}}{\partial t} + \frac{\partial (\alpha_{db} \rho_{db} u_m)}{\partial x} = F_r \tag{4}$$

Momentum Equations

m – Fluid:

$$\frac{\partial}{\partial t}\big((\alpha_m \rho_m + \alpha_{db}\rho_{db})u_m\big) + \frac{\partial}{\partial x}\big((\alpha_m \rho_m + \alpha_{db}\rho_{db})u_m^2\big) =$$

$$= -(\alpha_m + \alpha_{db})\frac{\partial p}{\partial x} - F_{ml}(u_m - u_l) - F_{mf}(u_m - u_f) +$$ (5)

$$+ Eu_l + F_r u_f + J\big(H[J]u_l - H[-J]u_m\big) + (\alpha_m \rho_m + \alpha_{db}\rho_{db})g$$

Liquid:

$$\frac{\partial}{\partial t}(\alpha_l \rho_l u_l) + \frac{\partial}{\partial x}(\alpha_l \rho_l u_l^2) = -\alpha_l \frac{\partial p}{\partial x} + F_{ml}(u_m - u_l) - F_{lf}(u_l - u_f) -$$

$$- Eu_l - J\big(H[J]u_l - H[-J]u_m\big) + \alpha_l \rho_l g$$ (6)

Fuel:

$$\frac{\partial}{\partial t}(\alpha_f \rho_f u_f) + \frac{\partial}{\partial x}(\alpha_f \rho_f u_f^2) = -\alpha_f \frac{\partial p}{\partial x} + \alpha_f \rho_f g - F_r u_f +$$

$$+ F_{mf}(u_m - u_f) + F_{lf}(u_l - u_f)$$ (7)

Energy equations

m – Fluid:

$$\frac{\partial}{\partial t}\big(\alpha_m \rho_m e_m + \alpha_{db}\rho_{db}e_{db}(T_m)\big) + \frac{\partial}{\partial x}\big[(\alpha_m \rho_m e_m + \alpha_{db}\rho_{db}e_{db}(T_m))u_m\big] =$$

$$= -P\left[\frac{\partial}{\partial t}(\alpha_m) + \frac{\partial}{\partial x}(\alpha_m u_m)\right] + Eh_l + Jh_l - R_{ms}(T_m - T_s) + \dot{Q}_{fm}$$ (8)

Liquid:

$$\frac{\partial}{\partial t}(\alpha_l \rho_l e_l) + \frac{\partial}{\partial x}(\alpha_l \rho_l e_l u_l) = -P\left[\frac{\partial}{\partial t}(\alpha_l) + \frac{\partial}{\partial x}(\alpha_l u_l)\right] -$$

$$- Eh_l - Jh_l + R_{ls}(T_l - T_s) + \dot{Q}_{fl}$$ (9)

Fuel:

$$\frac{\partial}{\partial t}(\alpha_f \rho_f e_f) + \frac{\partial}{\partial x}(\alpha_f \rho_f e_f u_f) = -\dot{Q}_{fm} - \dot{Q}_{fl}$$ (10)

Compatibility condition:

$$\alpha_m + \alpha_l + \alpha_f + \alpha_{db} = 1 \tag{11}$$

In the above equations, $H(J)$ is the Heaviside step function that becomes unity for positive values of the argument and zero otherwise. When $T_m < T_s$, the m-fluid is liquid and J is set to be zero and T_s is an "equivalent" interface temperature given by

$$T_s = \frac{R_{ms} T_m + R_{ls} T_l}{R_{ms} + R_{ls}} \tag{12}$$

When $T_m > T_s$, J is evaporation rate given by

$$J = \frac{1}{h_m - h_l} \left[R_{ms} (T_m - T_s) + R_{ls} (T_l - T_s) \right] \tag{13}$$

The water properties are calculated with a program developed in Kurchatov Institute [18].

2.1 The constitutive laws

The flow regimes are defined by the value of the void fraction: $\varphi \le 0.3$ (Bubbly), $0.3 < \varphi < 0.7$ (Churn-Turbulent), and $\varphi \ge 0.7$ (Droplet).

The exchange laws available for two-phase systems after making suitable modifications to account for the effect of a third phase are used. The presence of a third phase reduces the area concentration as the third phase must also share the same area. Therefore, the area concentration is modified by a factor Φ_{ij}; Φ_{ij} representing the effect of the phase k on the area concentration of phase i for its interaction with phase j.

$$\Phi_{ij} = \frac{\alpha_j}{\alpha_j + \alpha_k} \tag{14}$$

2.1.1 Interfacial Momentum Coupling

The interfacial momentum coupling is primarily due to drag. The drag force is based on Ishii and Zuber (1979). Specifically,

$$F_{ij} = \frac{3}{4} \alpha_i \Phi_{ij} \rho_j \frac{C_{Dij}}{l_i} |u_i - u_j| \tag{15}$$

where suffices i and j refer to dispersed and continuous phases, respectively. The drag coefficient for churn flow ($0.3 < \varphi < 0.7$) is defined by:

$$i = m, j = l, \quad C_{Dij} = \frac{8}{3} (1 - \varphi) \text{ and } l_i = 4 \cdot \left\{ \frac{g \Delta\rho}{\sigma} \right\}^{-1/2} \tag{16}$$

For dispersed flow

$$C_{Dij} = \frac{2}{3} l_i \left\{ \frac{g \Delta \rho}{\sigma} \right\}^{1/2} \cdot \left\{ \frac{1 + 17.67 (f(\varphi_i))^{6/7}}{18.67 f(\varphi_i)} \right\}^2 \tag{17}$$

where

$$\begin{aligned}
&i = m, \quad j = l, \quad \varphi \le 0.3 \quad f(\varphi_i) = (1 - \varphi)^{1.5} \\
&i = l, \quad j = m, \quad \varphi > 0.7 \quad f(\varphi_i) = \varphi^3 \\
&i = f, \quad j = m, l, \quad f(\varphi_i) = (1 - \alpha_f)^{1.5}
\end{aligned} \tag{18}$$

and l_i is obtained from

$$\frac{\rho_j |u_l - u_m|^2 l_i}{\sigma} = We_{cr} \begin{cases} 8 & \text{for} \quad i = m \\ 12 & \text{for} \quad i = l \end{cases} \tag{19}$$

2.1.2 Interfacial Heat Transfer and Phase Change

For $\varphi < 0.7$ heat transfer to liquid is estimated by superposition of radiation and film boiling heat fluxes. That is,

$$\dot{Q}_{fl} = n_f (h_r + h_c) \pi l_f^2 \Phi_{fl} (T_f - T_l) \tag{20}$$

where

$$n_f = \frac{6\alpha_f}{\pi l_f^3}, \qquad h_r = \sigma E_f \frac{T_f^4 - T_l^4}{T_f - T_l} \tag{21), (22}$$

and

$$h_c = 2.98 \cdot \left\{ \frac{\rho_m \lambda_m [h_{fm} + 0.68 c_{pm} (T_f - T_l)]}{l_f (T_f - T_l)} |u_f - u_l| \right\} \tag{23}$$

The emissivity value $E_f = 0.7$ is selected. Heat transfer from fuel to m-fluid in this regime need not be accounted for separately.

For $\varphi > 0.7$, a vapor-continuous regime in which heat is transferred to liquid drops by irradiation and to the gas (m-fluid) by convection is assumed. The m-fluid is allowed to superheat and convect heat to the liquid drops which boil at saturation. Thus:

$$\dot{Q}_{fl} = min(n_l \pi l_i^2, n_f \pi l_f^2) \sigma E_f E_l (T_f^4 - T_l^4) \tag{24}$$

and

$$\dot{Q}_{fm} = n_f \Phi_{fm} \pi l_f^2 h_c' (T_f - T_m) \tag{25}$$

where $n_l = 6\alpha_l \big/ \pi l_l^3$ and h_c' is given by

$$h_c' = \frac{\lambda_m}{l_f}\left\{2 + 0.6 \cdot Re_m^{1/2} \, Pr_m^{1/3}\right\} \tag{26}$$

where

$$Re_m = \frac{\rho_m \left|u_m - u_f\right| l_f}{\mu_m} \tag{27}$$

The factor E_l was introduced to empirically degrade the radiation heat transfer to liquid by the portion that could not be absorbed ($E_l = 0.3$).

Similarly, for vapor-to-liquid heat transfer we have:

For $\varphi < 0.7$, with vapor as the dispersed phase

$$R_{ls} = c_l n_m \Phi_{ml} \pi l_m^2 \frac{\lambda_l}{l_m}\left\{2 + 0.6\, Re^{1/2}\, Pr_l^{1/3}\right\} \tag{28}$$

$$R_{ms} = 2 n_m \Phi_{ml} \pi \, l_m^2 \, \frac{\lambda_m}{l_m} \tag{29}$$

while for $\varphi > 0.7$, with liquid (drops) as the dispersed phase

$$R_{ms} = n_l \Phi_{lm} \pi l_l^2 \frac{\lambda_m}{l_l}\left\{2 + 0.6\, Re^{1/2}\, Pr_m^{1/3}\right\} \tag{30}$$

$$R_{ls} = 2 c_l n_l \Phi_{lm} \pi \, l_l^2 \, \frac{\lambda_l}{l_l} \tag{31}$$

In the above equations the coefficient c_l was introduced as a way to control the liquid superheat in cases where these simplified formulations for heat transfer coefficients are not deemed adequate.

For the mass transfer from the fuel, the fragmentation rate, F_r , is calculated based on the instantaneous Bond number formulation.

The relevant equations are

$$F_r = \frac{6\alpha_f}{\pi l_f^3} \frac{dM}{dt} \tag{32}$$

where

$$\frac{dM}{dt} = \alpha_m \left(\frac{dM}{dt}\right)_m + (1 - \varphi_m)\left(\frac{dM}{dt}\right)_l \tag{33}$$

with

$$\left(\frac{dM}{dt}\right)_i = \frac{\pi l_f^2 |u_i - u_f|}{6 t_{b,i}^*} (\rho_f \rho_i)^{1/2} \quad for \quad i = m,l \tag{34}$$

φ_m is the "void fraction" of the m-fluid defined by

$$\varphi_m = \frac{\alpha_m}{\alpha_m + \alpha_l} \tag{35}$$

The "fragmentation time" and the instantaneous and Bond numbers for each phase are defined by

$$t_{b,i}^* = 13.8 Bo_i^{1/4} \quad and \quad Bo_i = \frac{3C_p \rho_i}{8\sigma} |u_i - u_f|^2 \frac{l_f}{2} \tag{36}$$

For the mass transfer between the m-fluid and liquid, the entrainment rate, E, is assumed to be directional proportional to the fragmentation rate. Specifically,

$$E = f_e F_r \frac{\rho_l}{\rho_f} \tag{37}$$

with f_e being an empirical entrainment factor which can be varied parametrically.

3   CALCULATION OF THERMAL DETONATION WAVE PROPAGATION

The partial differential equations are solved by a finite-difference method, which employs the usual staggered grid arrangement. All convective terms are approximated using upwind differencing. The semi-implicit procedure is used for calculation of the new time values of variables.

We have implemented a simulation of transient thermal detonation propagation in the corium-water mixture. The calculations were carried out under the following parameters:

Initial pressure   *0.1 MPa*
Initial fuel temperature   *3000 K*
Initial fuel volume fraction   *0.1*
Initial void fraction   *0.5*
Corium density   *8400* $kg \cdot m^{-3}$
Corium heat capacity *500* $J \cdot kg^{-1} \cdot K^{-1}$
Corium surface tension   *0.4* $N \cdot m^{-1}$
Initial drop size   *0.005 m*

Solution domain represents a closed vessel. Thus the only boundary condition is zero velocities at the vessel walls. To simulate triggering, a fraction of the fuel drops is fragmented in a small region near the bottom of the vessel. This causes a high heat transfer rate in these cells, the pressure rises locally and a detonation wave may develop.

Fig.1 shows calculated profiles of pressure and mixture velocities for subsequent moments. The length of the unsteady part of the wave propagation is about 3 m, the size of the fragmentation zone is about 0.3 m. Maximum pressure is about 500 MPa and maximum velocities are 470 m/s. Unsteady rarified wave is located near the fragmentation zone. Structure of steady-state thermal detonation wave is shown in Fig.2. Profiles of pressure and velocities of each phase are shown in Fig.2a, profiles of volume fractions of each phase are shown in Fig.2b, and temperature profiles and fragmentation rate are presented in Fig.2c.

Velocity equilibrium of liquid coolant and m-fluid occurs behind the detonation front at ~ 0.4 m. But the temperature of these phases does not practically change in the reaction zone and the liquid temperature keeps the initial value.

In work [12] the escalation of thermal detonation was calculated with assistance of mathematical model based on the traditional concept: the fragments were taken to mix homogeneously with the coolant (microinteractions did not take into account). Large escalation length (about 30 m) up to steady-state propagation stage has been obtained. Such value is essentially different compared with the results obtained in this paper (transient length about 3 m). The main reason for that is taking into account the microinteraction model.
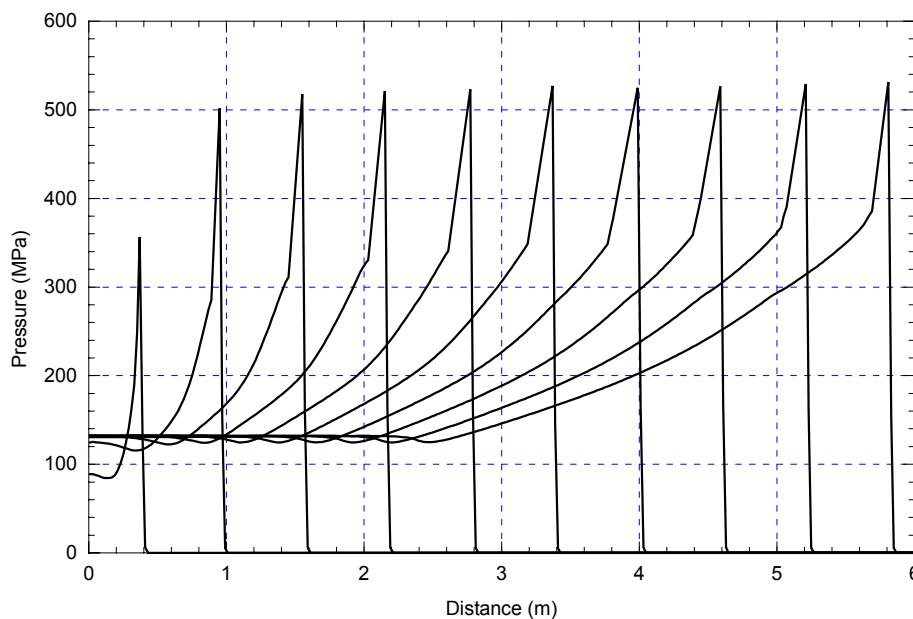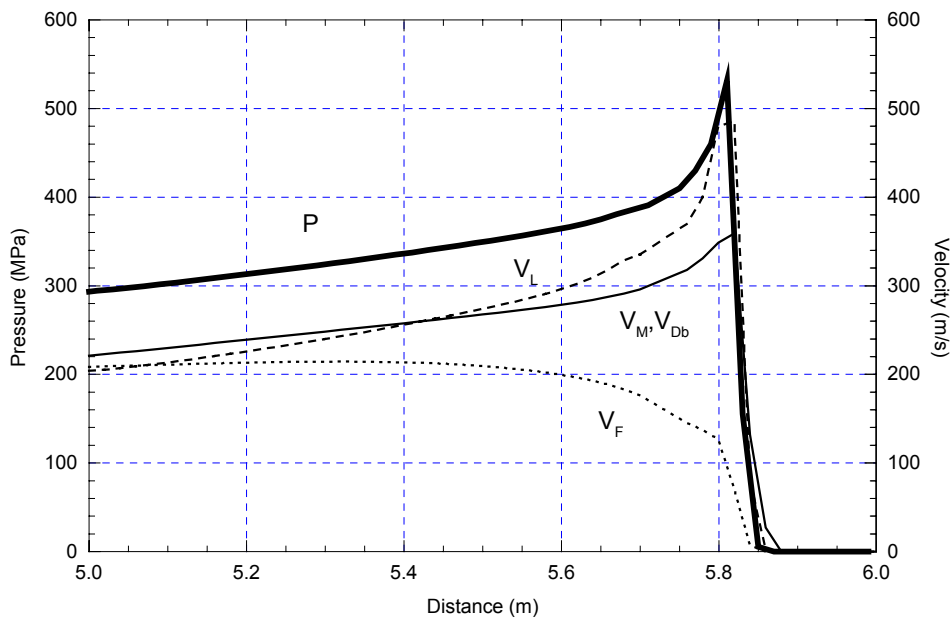

Figure 1a Escalation and propagation of thermal detonation wave in the corium-water mixture. Pressure profiles every 0.6 ms
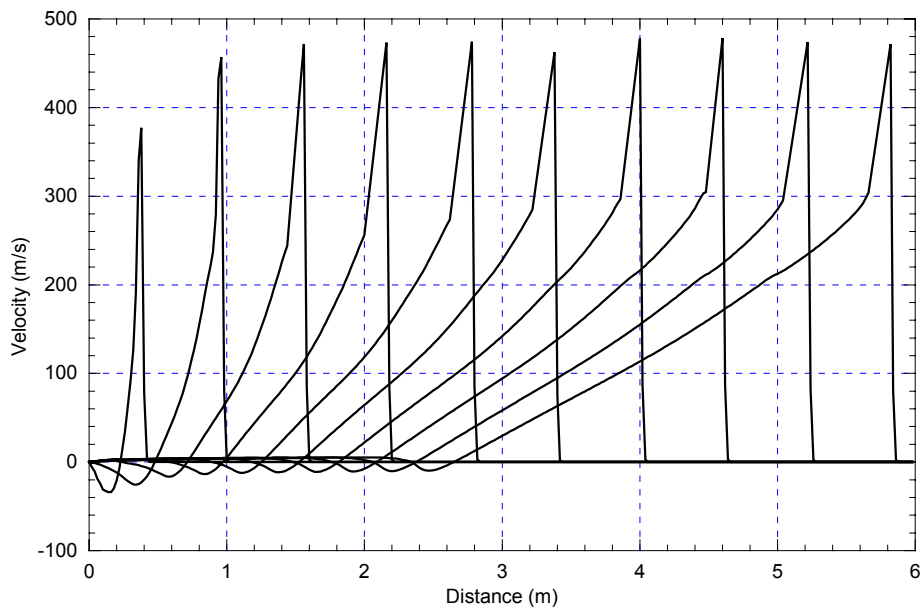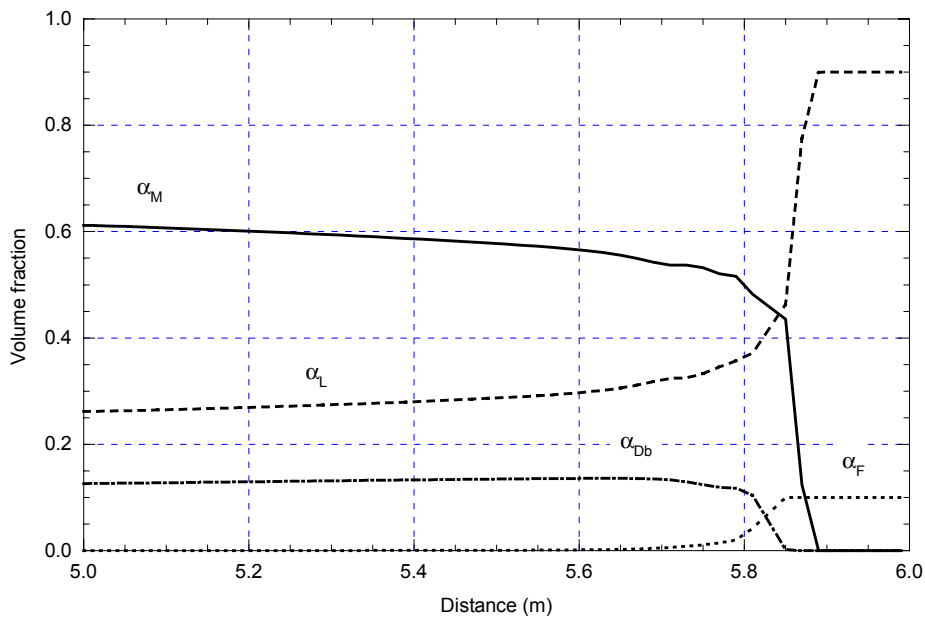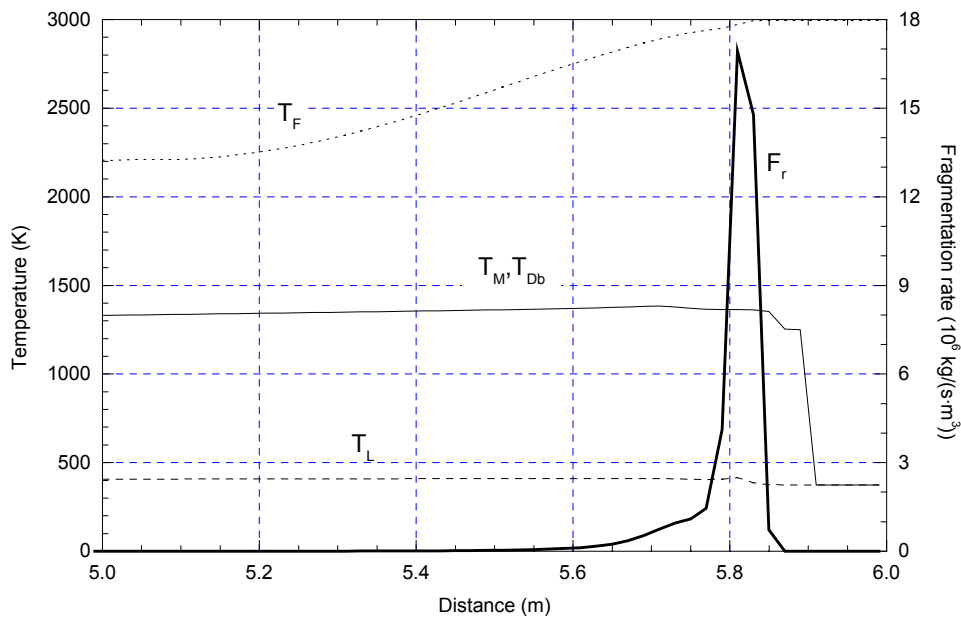
Figure 1b Escalation and propagation of thermal detonation wave in the corium-water mixture. Mixture velocity distribution

Figure 2a Structure of the thermal detonation wave. Distributions of the pressure and velocities of all phases

Figure 2b Structure of the thermal detonation wave. Distributions of the phase volume fractions

Figure 2c Structure of the thermal detonation wave. Distributions of the phase temperature and fragmentation rate

4   CONCLUSIONS

The thermal detonation taking into account microinteraction processes model has been applied to study thermal detonation wave escalation and propagation in the corium-water

mixture. Transient escalation stage and subsequent steady-state propagation stage of the thermal detonation have been calculated. The essential decrease of the escalation length (about 3m) in comparison with the previous results calculated without microinteraction concept has been obtained. So, one of conclusions of the work [12], that due to large escalation length for real reactor applications only non-steady thermal detonation models should be used, is not completely valid. Results of the present paper have shown the rapid approach to steady-state stage and therefore some estimations can be obtained with the assistance of the steady-state theory.

5   NOMENCLATURE

Bo *Bond number*
C_d *drag coefficient*
e *specific internal energy*
E *entrainment rate*
Fr *fragmentation rate*
F *factor for interfacial momentum exchange*
f_e *entrainment factor*
g *gravity*
h *specific enthalpy*
J *phase change rate*
l *length scale*
n *number of fuel particles (or liquid droplets) per unit volume*
p *pressure*
Pr *Prandtl number*
$\dot{Q}_{fm}$ *heat transfer rate between fuel and m-fluid*
$\dot{Q}_{fl}$ *heat transfer rate between fuel and liquid*
R_{ls} *heat transfer coefficient between the liquid and the liquid/m-fluid interface*
R_{ms} *heat transfer coefficient between the m-fluid and the liquid/m-fluid interface*
Re *Reynolds number*
t *time*
T *temperature*
t_b^* *fragmentation time*
u *velocity*

5.1   Greek

α *volume fraction*
λ *thermal conductivity*
ρ *density*
σ *surface tension or Stefan-Boltzman constant*
φ *void fraction*

5.2   Subscripts

db *debris*
f *fuel*

l   *liquid coolant*
m   *microinteraction fluid*
s   *saturation properties*

6   ACKNOWLEDGMENTS

7   REFERENCES

[1]   Berthoud, G.I. and Scott, E. "Multiphase Thermal Detonation for a $UO_2 - Na$ System," Proc. 4th CSNI Specialists Meeting on Fuel-Coolant Interaction in Nuclear Reactor Safety, Bournemouth, England, 2-5 April, 1979, 1, p.22 (1979).

[2]   Board, S.J., Hall, R.W. and Hall, R.S. "Detonation of Fuel Coolant Explosions," Nature, 254, 319 (1975).

[3]   Burger, M., Muller, K., Buck, M., Cho, S.H., Schatz, A., Schins, H., Zeyens, R., Hohmann, H. "Analysis of Thermal Detonation Experiments by Means of a Transient Multiphase Detonation Code," Proc. 4-th Int. Topical Meeting on Nucl. Reactor Thermal Hydraulics (NURETH-4), Karlsruhe, FRG, 10-13 October, 1989, 1, p.304 (1989).

[4]   Burger, M., Buck, M., Muller, K. and Schatz, A. "Stepwise Verification of Thermal Detonation Models: Examination by Means of the KROTOS Experiments," Proc. CSNI Specialists Meeting on Fuel-Coolant Interactions, Santa Barbara, USA, 5-8 January, 1993, p.218 (1994).

[5]   Carachalios, C., Burger, M. and Unger, H. "A Transient Two-Phase Model to Describe Thermal Detonations Based on Hydrodynamic Fragmentation," Proc. Int. Meeting on LWR Severe Accident Evaluation, Cambridge, Massachusetts, 28 August - 1 September, 1983,1, p.6.8.1 (1983).

[6]   Chen, X., Yuen, W.W. and Theofanous, T.G., "On the Constitutive Description of the Microinteractions Concept in Steam Explosions," Proc. 7-th Int. Meeting on Nucl. Reactor Thermal-Hydraulics (NURETH-7), Saratoga Springs, New York, 10-15 September, 1995, 3, p.1586 (1995).

[7]   Condiff, D.W. "Contributions Concerning Quasi-Steady Propagation of Thermal Detonations Through Dispersions of Hot Liquid Fuel in Cooler Volatile Liquid Coolants," Int. J.Heat Mass Transfer, 25, 87 (1982).

[8]   Fletcher, D.F." An Improved Mathematical Model of Melt-Water Detonations. 1. Model formulation and Example Results, "Int.J.Heat Mass Transfer, 34, 2435 (1991).

[9]   Fletcher, D.F. "Propagation Investigations using the CULDESAC Model," Proc. CSNI Specialists Meeting on Fuel-Coolant Interactions, Santa Barbara, USA, 5-8 January, 1993, p.180 (1994).

[10]   Gelfand, B.E., Bartenev, A.M. and Frolov, S.M. "Calculation of Explosive Interaction in the Melt-Coolant Mixture with a Thermal Detonation Model," Fizika Gorenia i Vzriva, 27, 6, 122 (1991) (in Russian).

[11]   Medhekar, S., Amarasooriya, W.H. and Theofanous, T.G. "Integrated Analysis of Steam Explosions," Proc. 4-th Int. Topical Meeting on Nucl. Reactor Thermal Hydraulics (NURETH-4), Karlsruhe, FRG, 10-13 October, 1989, 1, p.319 (1989).

[12]   Melikhov, O.I. and Melikhov, V.I. "Analysis of thermal detonation in the system "corium-water", Proceedings of the International Topical Meeting on Advanced Reactors Safety, June 1-5, 1997, Orlando, Florida, pp.496-502 (1997).

[13]   Okano, T. "One-dimensional Calculations of Melt/Water Detonations based on a Four-fluid Model," Proc. 2nd Int. Conf. on Multiphase Flow' 95-Kyoto, Kyoto, Japan, 3-7 April, 1995, 3, p.VE-19 (1995).

[14]   Scott, E. and Berthoud, G.I. "Multiphase Thermal Detonation," Topics in Two-Phase Heat Transfer and Flow, S.G.Bankoff (Ed.), p.11, ASME (1978).

[15]   Sharon, A. and Bankoff, S.G. "Propagation of Shock waves in a Fuel-Coolant Mixture," Topics in Two-Phase Heat Transfer and Flow, S.G.Bankoff (Ed.), p.51, ASME (1978).

[16]   Sharon, A. and Bankoff, S.G. "On the Existence of Steady Supercritical Plane Thermal Explosions," Int.J.Heat Mass Transfer, 24, 1561 (1981).

[17]   Theofanous, T.G., Yuen, W.W. "The Prediction of Dynamic Loads from Ex-vessel Steam Explosions," Proc. Int. Conf. "New Trends in Nucl. System Thermohydraulics, Pisa, Italy, 30 May-2 June, 1994, 2, p.257 (1994).

[18]   Nikonov, S.P., Nikonova, N.A. "Splain Approximation for a Calculation of Thermophysical Properties of Water and Steam," Report N32/1-2100-94, Kurchatov Institute, Moscow (1994) (in Russian).