



Contents lists available at ScienceDirect

Nuclear Engineering and Design

journal homepage: www.elsevier.com/locate/nucengdes



Theoretical study of flashing and water hammer in a supercritical water cycle during pressure drop

A.R. Imre^{a,*}, I.F. Barna^b, G. Ézsöl^b, G. Házi^a, T. Kraska^c

^a Simulator Laboratory, MTA KFKI Atomic Energy Research Institute, Budapest, POB 49, H-1525, Hungary

^b Thermohydraulics Laboratory, MTA KFKI Atomic Energy Research Institute, Budapest, POB 49, H-1525, Hungary

^c Institute for Physical Chemistry, University of Cologne, Luxemburger Str. 116, D-50939 Köln, Germany

ARTICLE INFO

Article history:

Received 9 November 2009

Received in revised form 22 January 2010

Accepted 1 March 2010

Available online xxx

ABSTRACT

During a loss of coolant accident (LOCA) the pressure of the coolant can drop significantly in the vicinity of the leak. It will be shown that unlike in pressurized water reactors (PWRs) where this pressure drop can cause only sudden vaporization – also called flashing – in supercritical water cooled reactors (SCWRs) it can cause sudden condensation (condensation-induced water hammer), too. The reason is that from supercritical state the system can go to metastable liquid as well as to metastable vapour state after LOCA. Relaxation from metastable fluid states is a fast process, followed by a local positive or negative pressure-jump, which might increase the damage around the leak. Conservative estimation will be given for the magnitude of these pressure jumps caused by the flashing or water hammer by assuming various initial pressure losses. In our calculations, three different equations of state are used: the simple van der Waals EoS; the Redlich–Kwong as an empirical development; and the more sophisticated non-cubic Deiters equation of state. These equations are able to describe metastable states qualitatively but with different accuracy. These calculations can help us to map the local immediate effect of any sudden pressure drop and therefore it can help to design better safety protocols.

© 2010 Elsevier B.V. All rights reserved.

1. Introduction

High temperature pressurized liquids can boil immediately upon releasing their pressure. The boiling usually happens when the pressure of the liquid reaches the equilibrium vapour pressure (also called saturation pressure), but sometimes it can happen at much lower values. In this latter case, the liquid will be metastable (superheated or stretched) for a short period of time before boiling, i.e. forming vapour bubbles. The sudden boiling (flashing) of a metastable liquid can be very fast, explosion-like process. In a similar vein, vapour (steam) can be overpressurized or undercooled to metastable vapour state before suddenly condensing, forming liquid droplets. In a pressurized water-loop – like the primary circuit of a pressurized water reactor (PWR) – the pressure can drop rapidly during a loss-of-coolant accident (LOCA), causing some metastable liquid and subsequently sudden vaporization or flashing. In the same system, metastable steam can be produced by the injection of cold liquid into the hot steam filled pipes (see water hammer). Just like in regular PWRs, the consequences of a LOCA have to be carefully studied in SCWRs too (Yi et al., 2004; Mori et al.,

2006; Ishiwatari et al., 2007). Since the proper design of Generation IV SCWRs is widely studied (Cheng and Yang, 2008; Ortega-Gómez et al., 2008; Fischer et al., 2009), background physical-chemistry calculations are more and more needed. In this paper, we are going to show the result of a theoretical investigation of the phase transition related effect of the pressure drop in an SCW-loop.

As a very simplified model, the cooling loop of an SCWR can be seen as a 25 MPa water-loop where the temperature changes between a minimal, subcritical and maximal, supercritical value (Fig. 1). Having a system like that, a sudden pressure drop can lead to an overheated liquid in some part of the system and an undercooled vapour in another part. This can cause a water hammer and flashing in different parts of the loop. In regular PWRs, the pressure drop (first pressure change) associated to the LOCA itself can cause only flashing, while for water hammer, injection of cold water is required. In SCWRs the cold water injection is not necessary for the sudden condensation causing water hammer. Both processes, flashing and water hammer, are associated with a sudden pressure change (second pressure change). Due to the fact that the initial LOCA itself is caused by some mechanical failure, these fast pressure changes can cause further damage in the already damaged structure. Therefore the knowledge of the highest possible pressure jumps is crucial for safety calculations.

The highest attainable level of metastability can give us an upper limit for the sudden pressure jumps caused by these two processes.

* Corresponding author.

E-mail address: imre@aeki.kfki.hu (A.R. Imre).

Nomenclature

LOCA	loss of coolant accident
SCWR	supercritical water cooled reactor
EoS	equation of state
PWR	pressurized water reactor
SCW	supercritical water
vdW	van der Waals
RK	Redlich–Kwong
D	Deiters
IAPWS	International Association for the Properties of Water and Steam

This level depends on a number of variables, including the purity of the liquid, the speed of the pressure or temperature change, etc. As a final limit, one can use the so-called mean-field spinodal, which is the thermodynamic stability limit where the isothermal compressibility of the system would turn into negative, causing instability (Debenedetti, 1996; Imre et al., 2002). These stability limits cannot be reached in liquid–vapour systems but they can be approached by changing the pressure/temperature very rapidly in a pure liquid or steam. Strictly speaking the spinodal is rather a diffusive stripe than a discrete curve as suggested by the so-called mean-field spinodal. However, the mean-field spinodal can be treated as very final limit of metastability.

The vapour spinodal is the limit where the vapour immediately has to turn into liquid. The liquid spinodal is the limit where the liquid has to boil immediately. Both can be easily calculated from an accurate equation of state (EoS) (Kraska, 2004; Abbasi and Abbasi, 2007; Jancsakar and Iványi, 2008). Unfortunately, most EoS cannot be used in the metastable region; this is particularly true for most of the reference EoSs, which are tuned only to describe stable liquid and vapour states and can produce several unphysical maxima, minima and divergences on the isotherms. For water, the so-called IAPWS (also called Wagner) EoS can be used to describe stable steam and liquid phases (Wagner and Pruss, 2002) but it cannot be used in the metastable region. Therefore we will use three other equations, which are less accurate but can be applied in the metastable region, too. By using these EoSs, we will give some estimation for the pressure jumps caused by the sudden vaporization or sudden condensation following a LOCA in a SCW-loop (SCW LOCA).

2. Models

2.1. Equation of states and spinodals

In our calculations, we used some assumptions to simplify the problem. The main assumption is that we are going to accept the validity of the EoS in the metastable region and we also accept that the equation, which can give us better results in the stable region, is probably also better in the metastable region. The second assumption is a simplification, namely instead of adiabatic changes, isotherm–isobar paths have been used. The third assumption is that we expect that the pressurized or stretched water jumps back only to the equilibrium value upon relaxing. For our calculations, the ThermoC code has been used (Deiters, 2006).

Concerning the first assumption, it is known that very sophisticated reference equation of states are completely inappropriate in the metastable region, giving several false stability limits, but – at least theoretically – the cubic equation of states and a few non-cubic ones can be used there. The second part of the first assumption is difficult to check, but at least one can assume that when an EoS gives worse result for the critical point (which is the final point of the spinodal lines) than probably the whole spinodal line will be worse

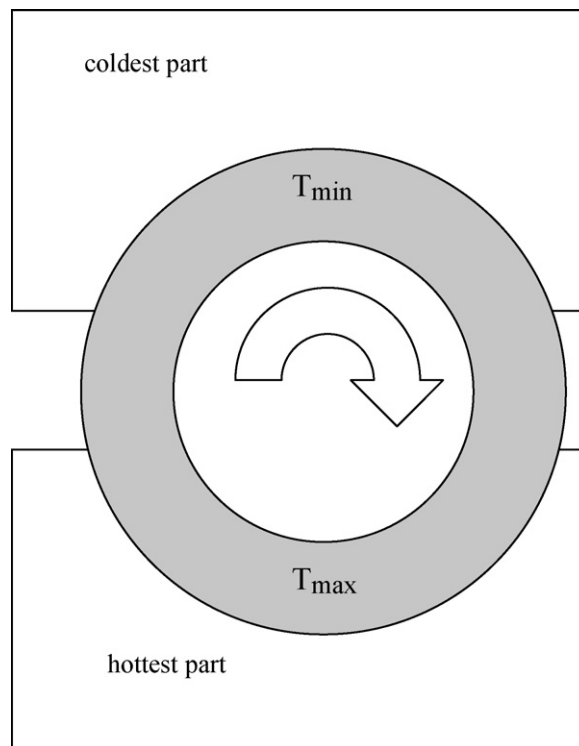


Fig. 1. A simplified, but topologically correct model of the cooling loop of an SCWR. The arrow marks the direction of the circulation.

and vice versa. In addition, it is known that the calculated spinodal is typically behind the experimentally obtained attainable stability limit for certain equations of state, which is consistent (Kraska, 2004).

Concerning the second assumption, the actual path for the initial pressure drop and temperature change (Fig. 2) to reach the stability line does not influence the final result (see later). Concerning the pressure jumps during phase transition (this is the second pressure change), due to the high speed, it is also accepted to approximate them with an isothermal path. Fast processes considered here are usually handled as adiabatic, not isotherm. In the liquid phase, the two paths are not very much different (adiabatic paths in the stud-

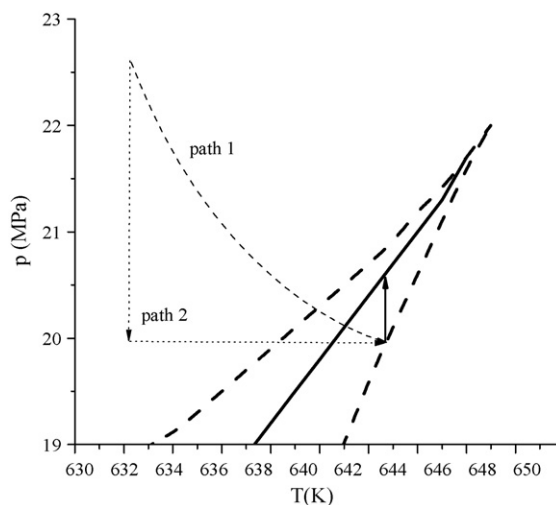


Fig. 2. Two different *pT*-paths starting from the same initial condition to reach the same point of the stability line (path 1 is a complex path, path 2 is a simplified isobar–isotherm one). The final pressure-jump (solid arrow) does not depend on the path.

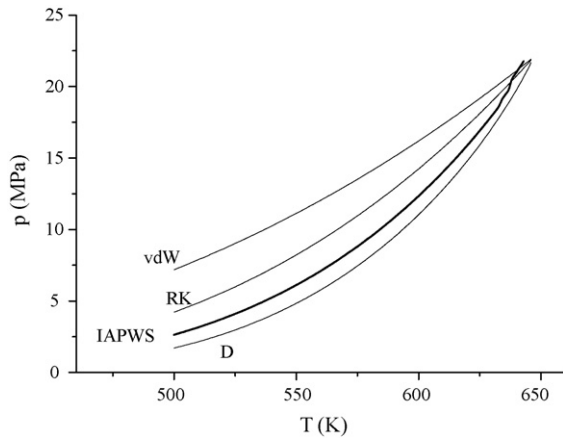


Fig. 3. Vapour pressure curves for water, calculated with various equation of states (vdW: van der Waals, RK: Redlich–Kwong, IAPWS: Wagner–Pruss, and D: Deiters).

ied conditions would be associated with a 1–2 K shifts), but in the vapour phase isothermal and adiabatic paths are quite different. In our studies, isothermal paths were considered for two reasons. First, experimental results suggest (see, for example, Barten et al., 2008) that the pressure and temperature changes associated with LOCA is neither isothermal, nor adiabatic, but still much closer to an isotherm. RELAP5 calculations suggested approx. 100 K temperature increase (using adiabatic model), while the measured change was only 5–8 K.

The third assumption of incompressible liquid water is not really good but we can use it to get some conservative estimate.

The three EoSs used in our calculations are the classical van der Waals (vdW) equation of state (van der Waals, 1910), the Redlich–Kwong (RK) equation of state (Redlich and Kwong, 1949) and the Deiters (D) equation of state (Deiters, 1981a,b, 1983). The vdW-EoS is the oldest cubic equation of state, quite inaccurate and mainly historically and topologically interesting. The RK-EoS is an empirical extension of the vdW-EoS used mainly at higher temperatures, but not yet very good for water. The D-EoS is non-cubic and exhibits quite fair result for water. To check the accuracy of these EoSs, we are calculating the vapour pressure and compare it to the value given by the IAPWS-95 reference equation. The results, calculated by the ThermoC program (Deiters, 2006), using the built-in parameters for water, can be seen in Fig. 3. The vapour pressure curve given by the van der Waals equation differs from the IAPWS to a great extent, the D-EoS predicts the vapour pressure curve fairly well, while the difference by the RK-EoS – just as we expected – is between the two others. As an example, we show the vapour pressures at 500 K: for the IAPWS reference EoS it is 2.63 MPa, for the vdW EoS it is 7.19 MPa (+4.56 MPa difference), for the RK EoS it is 4.21 MPa (1.58 MPa difference), and finally for the D-EoS it is 1.71 MPa (0.92 MPa difference).

In Fig. 4 the fluid–fluid phase- and stability diagram is shown in the vicinity of the critical point calculated by the three different EoSs. Solid lines mark the vapour pressure curves; dashed curves mark the liquid–vapour spinodal where the metastable liquid must turn into vapour; the dotted curves mark the vapour–liquid spinodal where the metastable vapour must turn into liquid; the grey dot-dash is the so-called Widom-line or pseudospinodal (Stanley et al., 2008), which is a diffuse border between the liquid-like SCW and the vapour-like SCW; and finally the upper short-dashed curves mark the normal working condition of the water in an SCWR. The vapour pressure curve, the two spinodals and the Widom-line meet in the critical point. The Widom-line is the line where the compressibility of the SCW has a maximum. The region around the Widom-line is the zone, where most properties of the SCW change

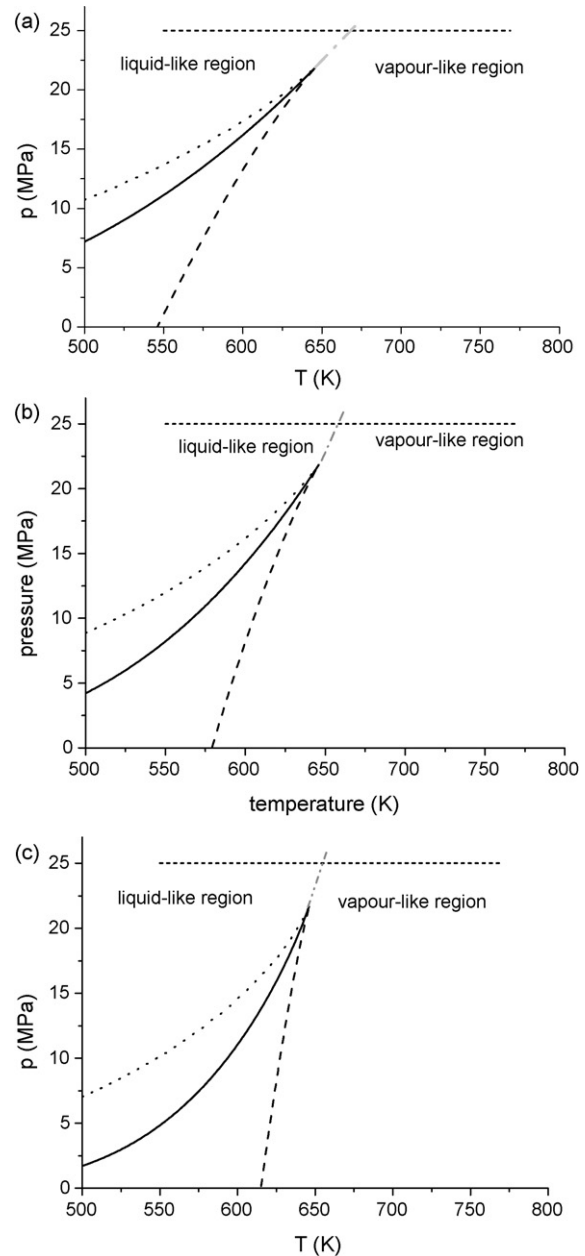


Fig. 4. Vapour pressure curves (solid), liquid–vapour spinodals (dashed), vapour–liquid spinodals (dotted), and pseudospinodals (grey dot-dashed) for water, calculated with van der Waals (a), Redlich–Kwong (b) and Deiters (c) equation of states. Short-dashed lines mark the normal working condition of the water in an SCWR.

rapidly. At temperatures below the Widom-line the SCW is more liquid-like, where at temperatures above it the SCW is more like a vapour, concerning several relevant chemical and physical properties.

3. LOCA in an SCWR loop

We use here an unstructured water-loop (i.e. a ring-formed closed pipe without pressurizer) as model, where the initial pressure is 25 MPa and the temperature at one part 551 K, changing smoothly to 769 K at the opposite side of the circle (Fig. 1). When pipe breaks, we assume an immediate pressure loss at the vicinity of the breaking point. We calculate two cases, locating the breaks into the two temperature extrema. The pressure loss will spread along

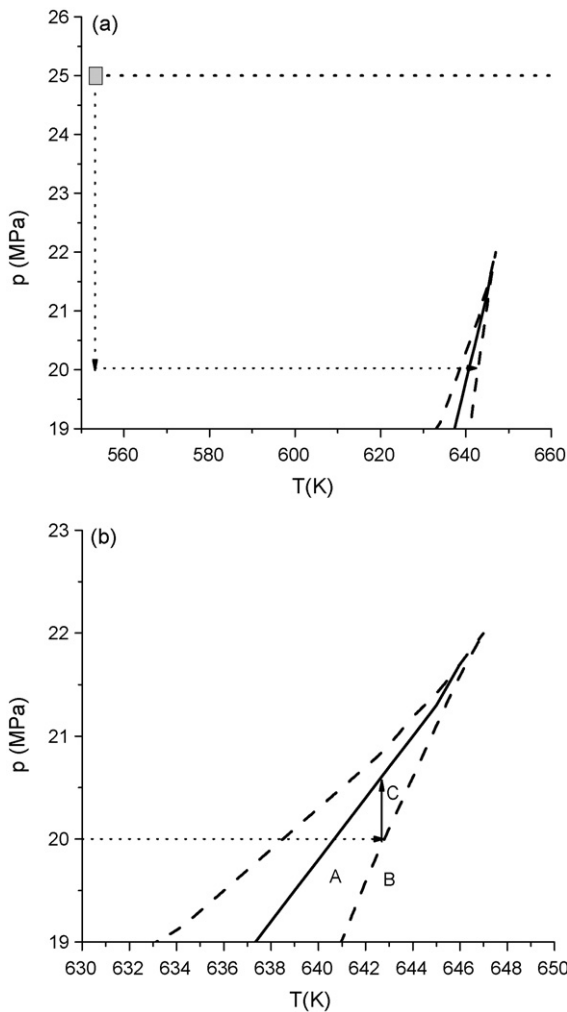


Fig. 5. The effect of a 5 MPa pressure drop in the low-temperature side of a SCW-loop, figure (b) is the magnification of figure (a). Short-dashed line mark the normal working condition of the water in an SCWR, grey square marks the initial condition of the LOCA, dashed lines are the spinodals, solid line is the vapour pressure curve. Dotted line marks the isotherm pressure drop, the isobaric heating of the water and finally the sudden pressure-jump caused by the vaporization. Full description can be seen in the text.

the loop. In Fig. 5 one can see the effect of a pressure drop caused by a LOCA in the region where the SCW is more liquid-like (i.e. at lower temperatures, below $T_{\text{Widom}}(25 \text{ MPa}) \approx 658 \text{ K} \approx 385 \text{ }^\circ\text{C}$). In Fig. 6, the same process can be seen on the high-temperature side. In both figures, part (b) is a magnification of the region of sudden boiling or condensation.

The whole process is demonstrated in Figs. 5 and 6. In Fig. 5, one can see a sudden pressure drop from 25 to 20 MPa (down-side dotted arrow), starting from the initial condition, marked by grey square). A 5 MPa pressure drop resembles to a small or medium break LOCA in PWR, but because the density and compressibility of supercritical water are much smaller than for the subcritical water, a geometrically identical leak can cause smaller and/or slower pressure drop in SCWR loops. Therefore, 5 MPa might be caused by a medium or large break SCWR-LOCA too. This drop happens in the low-temperature part of the SCW-loop, but then – due to the permanent loss of pressurized fluid – this “low-pressure” zone will expand into the higher temperature region (vertical dotted arrows). It should be noted that the arrows are a simplified path while the real path is not linear, i.e. not isothermal nor isobaric. On the other hand, the path from the initial condition to point B does not influence the magnitude of the B-to-C jump, therefore it is

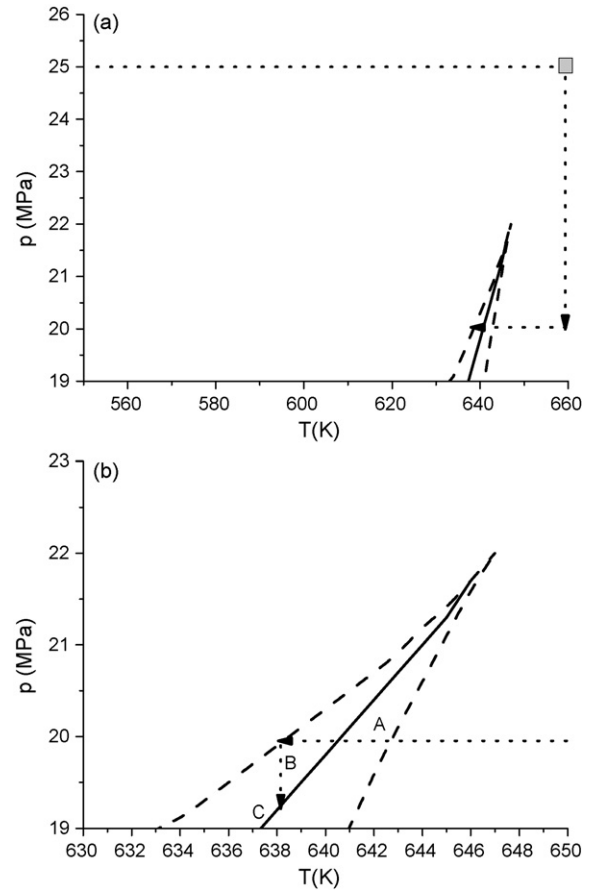


Fig. 6. The effect of a 5 MPa pressure drop on the high-temperature side of a SCW-loop, (b) is the magnification of (a). Further description can be seen in Fig. 5 and in the text.

irrelevant. Crossing the vapour pressure line (point A) the already liquid water will be metastable (superheated). In the vicinity of the liquid–vapour spinodal (point B) the extremely high level of metastability has to cause sudden boiling, causing pressure-jump (upward dotted arrow). After a transient pressure peak – neglected in our model – the system will be more or less equilibrated at the vapour pressure (point C).

In Fig. 6, one can see a similar pressure drop (long downward dotted arrow), happening in the high-temperature region. The low-pressure zone will expand into the direction of low-temperature region. Crossing the vapour pressure line (point A) the already vaporized water will be metastable steam. In the vicinity of the vapour–liquid spinodal (point B) it has to condensate, causing a pressure drop (short downward arrow). After the neglected transient pressure peak, the system will be more or less equilibrated at the vapour pressure (point C).

In Fig. 7, one can see the absolute value of the pressure differences before and after the sudden vaporization or condensation ($\text{abs}(p(C)-p(B))$), following various initial pressure drop (starting from 25 MPa), calculated by the vdW-, RK- and D-EoS. The solid lines are associated with the sudden vaporization, the dashed ones are associated with the sudden condensation. As one can see, the pressure-jump associated with the sudden phase transitions are as big as several MPa. Thus surely enough can cause some problems for the already damaged pipe walls. Jumps calculated by the D-EoS are approximately 50% higher than by the ones calculated by the vdW-EoS; this can demonstrate the necessity to use a more accurate EoS. For initial pressure drops below approx. 3 MPa (which is equal with the difference of the working and critical pressures), sudden con-

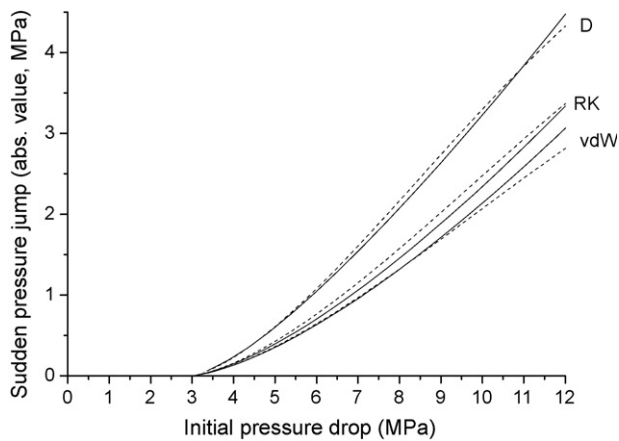


Fig. 7. The absolute magnitude of the sudden pressure change ($\text{abs}(p(C)-p(B))$), associated with sudden boiling or condensation following SCW LOCA, calculated by van der Waals and by Deiters equation of states.

condensation cannot be seen, because the water still remains above the critical pressure and the temperature change itself cannot induce phase transition. We should remark here that in our previous report (Imre et al., 2009b), the pressure jumps associated to the sudden condensation were underestimated; the correct values are reported here.

We should mention here, that any deviation from the isothermicity to the direction of adiabacity (Barten et al., 2008) would shift point C (Fig. 6/b) higher on the vapour pressure curve, causing smaller $p(B)-p(C)$ jump. Therefore isotherm path still can be used to find upper limit for the jump.

One can see that for initial pressure drops smaller than approx. 3 MPa, nothing happens. This is due to the lack of phase transition above the critical point. In this vein, we could propose that for SCW-loops, where the normal working pressure are higher, one can have a safety pressure drop range where both phenomena can be avoided and which can be increased by increasing the working pressure (in case of 30 MPa working pressure it would be an 8 MPa range). Therefore the increase of the working pressure would be a possible way to avoid LOCA-related phase transitions in SCWRs.

Another way to avoid sudden boiling or condensation would be the prevention of the extension of the low pressure zone. In Fig. 8, one can see that by stopping the “negative” pressure wave before reaching the vapour pressure curve (at point A, before reaching point B) by properly inserting one or more pressurizer, one could avoid the phase transition.

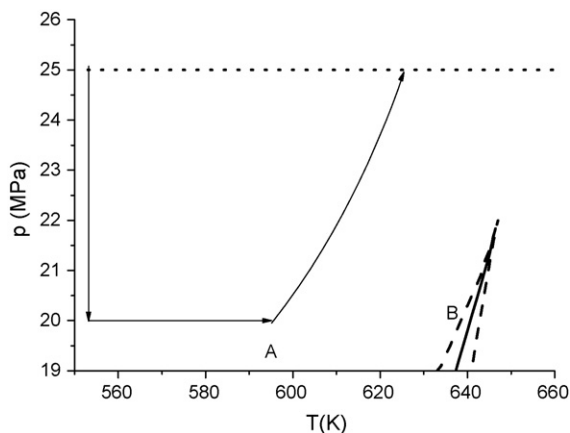


Fig. 8. A possible pressure-temperature route to avoid phase transition following SCW LOCA.

Sudden condensation is only a necessary but not sufficient condition for water hammer. In subcritical water + steam systems there are various thermal, hydraulic, geometrical, etc. conditions which have to be fulfilled to obtain water hammer. These conditions are the following (Griffith, 1997):

- the pipe must be almost horizontal;
- the subcooling must be greater than 20 °C;
- the length/diameter must be above 24;
- the velocity must be low enough;
- there should be a void nearby;
- the pressure must be high enough so that significant damage occurs.

From these conditions, only point “b” and “e” is necessary to obtain sudden condensation, the other four are needed to turn this condensation to damaging water hammer. For SCW-loops, a similar set of conditions will be necessary to obtain a water hammer; some of them might be similar but some of them will be certainly different. The extent of necessary subcooling to obtain metastability and sudden condensation is temperature-dependent (Imre et al., 2002; Imre et al., 2008; Kraska, 2004), close to the critical point the whole metastable region can be narrower than 20 °C, therefore for SCWRs (where the temperatures are much higher than for PWRs) point “b” probably should be modified. Point “e” declares the presence of a vapour void; in SCWR loops, this will not be necessary, being the whole system “vapour-like”. To find the necessary conditions to obtain a water hammer in an SCW-loop, further and detailed studies will be needed; some of them are already in progress.

4. Summary

We have analyzed the aftermath of a sudden pressure loss (e.g. LOCA) in a simplified SCW-loop. Depending on the location of the pressure loss (leak), the initial pressure drop can cause sudden boiling (flashing) or sudden condensation (water hammer). Using three different equation of states (van der Waals, Redlich–Kwong and Deiters) we calculated the pressure change caused by the phase transition as the function of the initial pressure drop. Using the same assumptions, an initial 10 MPa pressure drop caused a secondary pressure drop/jump during water hammer or flashing: approx. 2.1 MPa with vdW-EoS, 2.6 MPa with RK-EoS and finally approx. 3.1 MPa by D-EoS. The differences demonstrate the necessity to find a good EoS or any other method to calculate spinodals (Imre et al., 2008; Imre and Kraska, 2008; Imre et al., 2009). Finally, we tried to indicate how to avoid the phase transition, which can cause further damage in the already damaged pipes.

Acknowledgements

This work was supported by National Office for Research and Technology under the grant NUKENERG2. A.R. Imre was supported by Hungarian Research Fund (OTKA) under contract No. K67930 and the German Humboldt Foundation. The authors wish to thank the helpful advice of Prof. I. Tiselj (Slovenia).

References

Abbasi, T., Abbasi, S.A., 2007. Accidental risk of superheated liquids and a framework for predicting the superheat limit. *Journal of Loss Prevention in the Process Industries* 20, 165–181.

Barten, W., Jasiulevicius, A., Manera, A., Macian-Juan, R., Zerkak, O., 2008. Analysis of the capability of system codes to model cavitation water hammers: simulation of UMSICHT water hammer experiments with TRACE and RELAP5. *Nuclear Engineering and Design*, 1129–1145.

Cheng, X., Yang, Y.H., 2008. A point-hydraulics model for flow stability analysis. *Nuclear Engineering and Design* 238, 188–199.

- Debenedetti, P.G., 1996. *Metastable Liquids: Fundamentals and Applications*. Princeton University Press.
- Deiters, U.K., 1981a. A new semiempirical equation of state for fluids. I. Derivation. *Chemical and Engineering Science* 36, 1139–1146.
- Deiters, U.K., 1981b. A new semiempirical equation of state for fluids. II. Application to pure substances. *Chemical and Engineering Science* 36, 1146–1151.
- Deiters, U.K., 1983. Calculation and prediction of fluid phase equilibria from an equation of state. *Fluid Phase Equilibria* 10, 173–182.
- Deiters, U.K., 2006. ThermoC, <http://thermoc.uni-koeln.de/index.html>.
- Fischer, K., Schulenberg, T., Laurien, E., 2009. Design of a supercritical water-cooled reactor with a three-pass core arrangement. *Nuclear Engineering and Design* 239, 800–812.
- Griffith, P., 1997. *Screening Reactor Steam/Water Piping systems for Water Hammer*, NUREG/CR-6519.
- Imre, A.R., Maris, H.J., Williams, P.R. (Eds.), 2002. *Liquids Under Negative Pressure*, NATO Science Series. Kluwer, Dordrecht.
- Imre, A.R., Mayer, G., Házi, G., Rozas, R., Kraska, T., 2008. Estimation of the liquid–vapor spinodal from interfacial properties obtained from molecular dynamics and lattice Boltzmann simulations. *Journal of Chemical Physics* 128, 114708.
- Imre, A.R., Kraska, T., 2008. Liquid–vapour spinodal of pure helium-4. *Physica B* 403, 3663–3666.
- Imre, A.R., Házi, G., Kraska, T., 2009a. Estimation of the explosive boiling limit of metastable liquids. In: Rzoska, S.J., Mazur, V.A. (Eds.), *NATO Science Series: Metastable Systems Under Pressure: Platform for New Technologies and Environmental Applications*. Springer, pp. 271–278.
- Imre, A.R., Barna, I.F., Farkas, I., Márkus, A., Házi, G., Kraska, T., 2009b. Theoretical investigation of sudden vaporization and water hammer in SCWR during Loss of Coolant Accidents. In: *Proceeding of the 4th International Symposium on Supercritical Water-Cooled Reactors*, Paper No. 14.(CD).
- Ishiwatari, Y., Oka, Y., Koshizuka, S., 2007. Safety of the super LWR. *Nuclear Engineering and Technology* 39, 257–272.
- Jancsár, I., Iványi, A., 2008. Phenomenological hysteresis model for vapor–liquid phase transitions. *Pollack Periodica* 3, 5–28.
- Kraska, T., 2004. Stability limit of pure substances: an investigation based on equation of state. *Industrial & Engineering Chemistry* 43, 6213–6221.
- Mori, M., Maschek, W., Rineiski, A., 2006. Heterogeneous cores for improved safety performance: A case study: the supercritical water fast reactor. *Nuclear Engineering and Design* 236, 1573–1579.
- Ortega-Gómez, T., Class, A., Lahey Jr., R.T., Schulenberg, T., 2008. Stability analysis of a uniformly heated channel with supercritical water. *Nuclear Engineering and Design* 238, 1930–1939.
- Redlich, O., Kwong, J.N.S., 1949. On the thermodynamics of solutions. V. An equation of state. Fugacities of gaseous solutions. *Chemical Reviews* 44, 233–244.
- Stanley, H.E., Kumar, P., Franzese, G., Xu, L., Yan, Z., Mazza, M.G., Buldyrev, S.V., Chen, S.H., Mallamace, F., 2008. Liquid polyamorphism: possible relation to the anomalous behaviour of water. *European Physical Journal* 161, 1–17.
- van der Waals, J.D., 1910. *The Equation of State for Gases and Liquids*, Nobel Lecture, http://nobelprize.org/nobel_prizes/physics/laureates/1910/waals-lecture.pdf (12.12.1910).
- Wagner, W., Pruss, A., 2002. The IAPWS formulation 1995 for the thermodynamic properties of ordinary water substance for general and scientific use. *Journal of Physical and Chemical Reference Data* 31, 387–535.
- Yi, T.T., Ishiwatari, Y., Koshizuka, S., Oka, Y., 2004. Startup thermal analysis of a high-temperature supercritical-pressure light water reactor. *Journal of Nuclear Science and Technology* 41, 790–801.