Modification and Application of the ATHLET-SC Code to Trans-critical Simulations

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Abstract

In the simulation of trans-critical transients of Supercritical water cooled reactor (SCWR), calculation will terminate because of the sudden change in void fraction across the critical point. To solve this problem, a pseudo two-phase method is proposed with a virtual region of latent heat at pseudo-critical temperatures. A smooth variation of void fraction can be realized by using liquid-field conservation equations at temperatures lower than the pseudo-critical temperature, and vapor-field conservation equations at temperatures higher than the pseudo-critical temperature. Using this method, the system code ATHLET is modified to ATHLET-SC mod 2 on the basic of the previous modified version ATHLET-SC by Shanghai Jiao Tong University. The results of tests are verified that the calculation error with the pseudo two-phase method for supercritical fluid is acceptable, when the virtual region of latent heat is kept small. Moreover, the ATHLET-SC mod 2 code is used to simulate the pressurization and depressurization process of a single flow channel with the pressure transition as well as blowdown process. The results indicate a good applicability of the modified code.

Keywords: Pseudo two-phase method; Trans-critical transient; ATHLET-SC

1. Introduction

As the combination of the two mature technologies, modern commercial light water reactor and supercritical fossil-fired power plant, supercritical-pressure water cooled reactor (SCWR) is now receiving worldwide attention. It has shown considerable advantages in system simplification, thermal efficiency increase, construction and generation cost reduction [1]. Looking into the ongoing research work on SCWR in the world, satisfying fruits have achieved by the R&D efforts. The scope has covered SCWR nuclear system conceptual design, fundamental thermal-hydraulic research, key material characteristics research, numerical simulation and analysis codes development as well as safety analysis. Nevertheless, systematic research on the safety system of SCWR has not been deeply carried out up to now. Restricted by this deficiency, safety analysis mainly focuses on modifying the existing system analysis codes-which have been extensively used for LWR (e.g. RELAP)-to make it available to SCWR, and developing simplified thermal-hydraulic analysis codes [2].

Similar to pressure water reactor (PWR)， the loss of coolant accident analysis play a very important role in the safety analysis of SCWR. During the loss of coolant accident, single-phase state of the coolant will suddenly change into two-phase state by the fast transition from supercritical to subcritical pressure. Therefore, how to achieve the trans-critical simulation is the key point for the development of SCWR thermal-hydraulic analysis codes. Considering the current research status worldwide, a LOCA analysis code named SCRELA for supercritical-pressure water cooled reactors is developed by J.H. Lee, et al., and a large break LOCA of the thermal neutron spectrum reactor is analysed [3], but SCRELA uses the homogenous equilibrium model for the simulation of fluid-dynamics, and the homogenous equilibrium model is seldom sufficient for the calculation of two-phase flow below the critical pressure; the APROS system code [4] which is developed by Markku.H, et al. and bases on two-fluid model can simulate the trans-critical transition, but because of its simple function, APROS only can simulate simple system analysis of SCWR. To solve these problems, a pseudo two-phase method is used to modify ATHLET code, which is based on 5-equation model & two-fluid model. This method can be applied to the advanced best-estimate code for the safety analysis of light water reactor.

2. Modification of the ATHLET-SC

The thermal-hydraulic computer code ATHLET is being developed by the Gesellschaft für Anlagenund Reaktorsicherheit (GRS) for the analysis of design basis and beyond design basis accidents in light water reactors. The ATHLET structure is highly modular. It provides a modular network approach for the representation of a thermal-hydraulic system by using its basic modules [5].

ATHLET offers the possibility of choosing between different models for the simulation of fluid-dynamics [4]:

[1] 5-equation model, with separate conservation equations for liquid and vapor mass and energy, and a mixture momentum equation, accounting for thermal and mechanical non-equilibrium, and including a mixture level tracking capability,

[2] two-fluid model, with separate conservation equations for liquid and vapor mass, energy, and momentum (without mixture level tracking capability).

In order to extend the code's application range to the safety analysis under supercritical-pressure condition, a supercritical water thermo-physical property package is implemented into ATHLET 2.1 cycle A to take place the existing water-steam property package [6]. But ATHLET-SC only offers liquid mass, energy and momentum equation for the simulation of fluid-dynamics under supercritical-pressure condition. And the current version of the code cannot simulate the trans-critical process which indicates the transition between supercritical and subcritical pressure.

2.1 Pseudo two-phase method

In subcritical pressure, there is a saturated region for water, where gas and liquid simultaneously exist. With the transition between gas and liquid in this region, the fluid temperature keeps the same, and void fraction varies between 0 and 1. But when the fluid pressure above the critical pressure (greater than 22.064MPa), the fluid has only single-phase state, so there is no saturation of supercritical fluid temperature and void fraction in this state. Therefore the change in void fraction of fluid is not continuous during the trans-critical process. The discontinuous change of void fraction will directly affect the numerical calculation of two-fluid model, and cause calculation errors. In order to avoid discontinuous change of void fraction in the trans-critical process, a pseudo two-phase method is introduced with a virtual region of latent heat at pseudo-critical temperatures (heat capacity C_P is maximized at this temperature). This paper presents a pseudo two-phase method to approximate the fluid under supercritical pressure. Using this method, the system code ATHLET is modified to ATHLET-SC mod 2 on the basic of the previous modified version ATHLET-SC. In this method, the virtual saturated region built based on the pseudo-critical line which is an extension of the saturation curve to the supercritical pressure region (see in Figure 1). The temperature of the fluid in this region maintained at pseudo-critical temperatures, and the pseudo-saturation enthalpies are then set to

$$h_f^{\sup} = h_{p-critical} - 0.5h_{fg}^* \tag{1}$$

$$h_g^{\sup} = h_{p-critical} + 0.5h_{fg}^* \tag{2}$$

The enthalpy of vaporization keeps as a constant which is determined by the pressure below the SC point. If the pressure is much closed to the SC pressure, the h_{fg}^* will be small. The calculation will appear disturbed through the region, and the calculation time step will be required less. But the errors of the pseudo two-phase method will be small. On the contrary, if the pressure is far from the SC pressure, the h_{fg}^* will be larger, and the errors of the pseudo two-phase method will be larger. But the disturbed of the calculated results will be smaller. the limit of the calculation time step will be expanded. To balance above two factors, it is set as the value under 22.06MPa in this paper. So a smooth variation of void fraction can be realized by using liquid-field conservation equations at enthalpy lower than h_f^{sup}, and vapor-field conservation equations at enthalpy higher than h_g^{sup}.

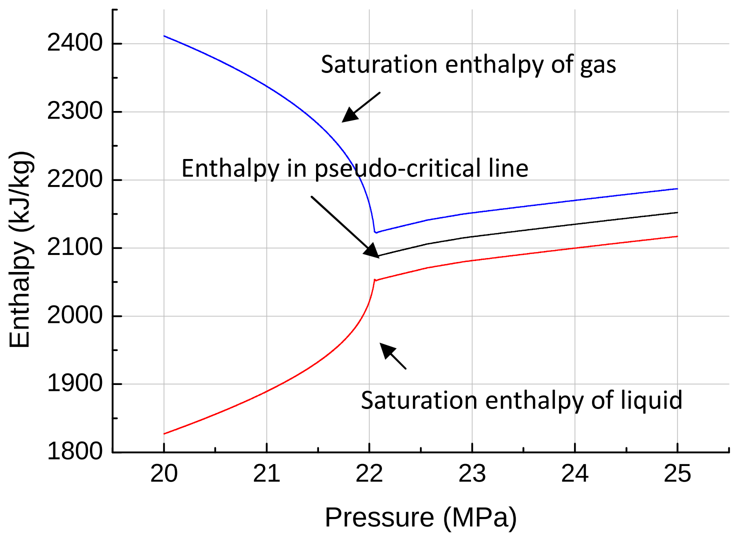


Figure 1 Saturation enthalpies of gas and liquid

2.2 Calculation of pseudo-critical temperatures

The key point of the Pseudo two-phase method is identification of pseudo-critical temperature and enthalpy. As show in Figure 2, thermodynamic properties of water (such as specific volume, enthalpy, etc.) change with temperature increase near the pseudo critical temperature. And enthalpy is calculated by pressure and temperature in normal way. A small error of the pseudo critical temperature will contribute to large uncertainty of the pseudo critical enthalpy, as show in Figure 3. Therefore, pseudo critical temperature must be calculated with high precision. This paper has developed a fitting equation for the fast calculation of pseudo critical temperature with good precision. This fitting equation can be used to calculate pseudo critical temperature within the pressure range of 22.064-30MPa.

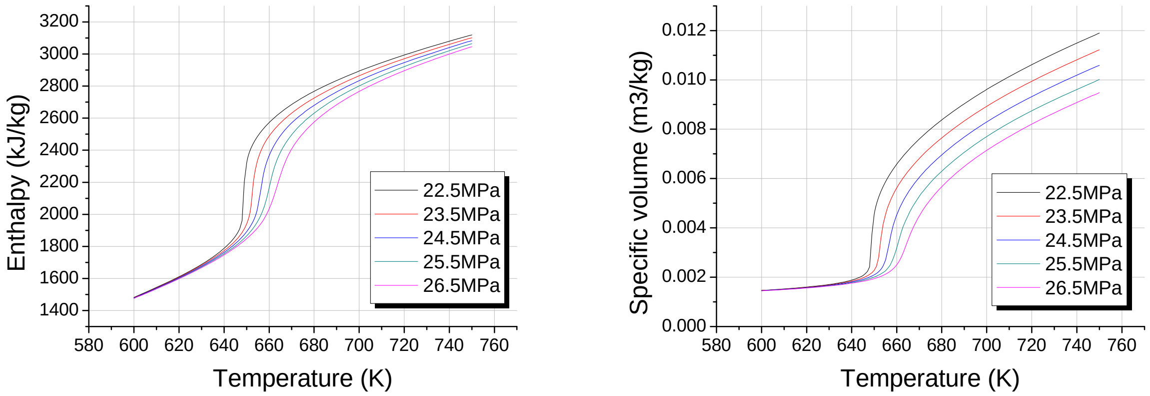
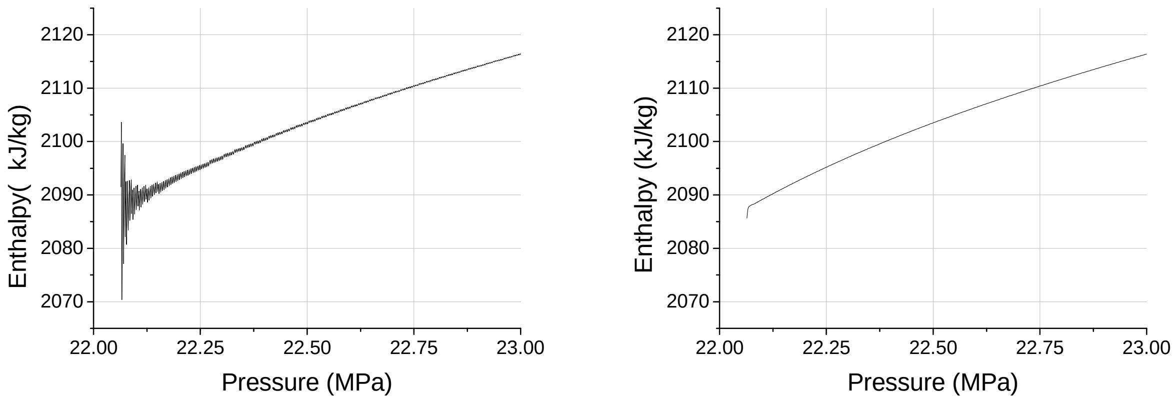
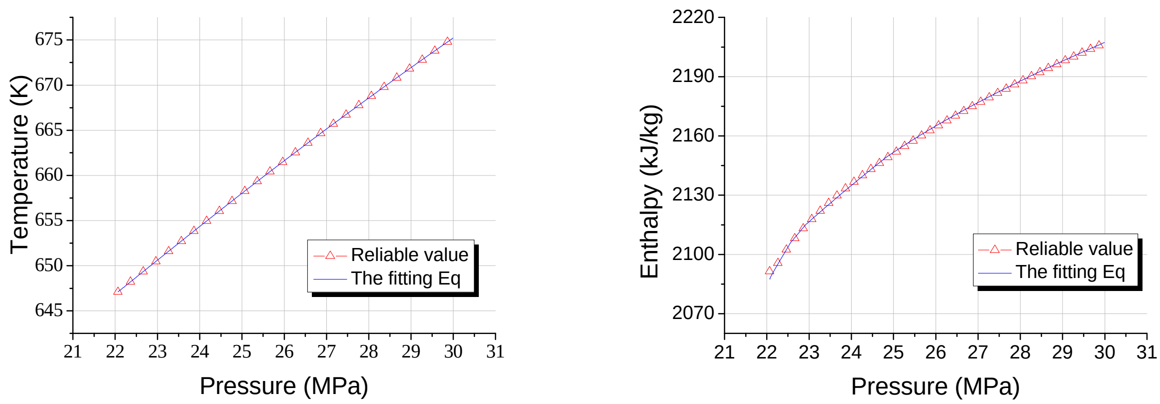


Figure 2 Change of properties with temperature



[A] Lower precision [B] Higher precision

Figure 3 Change of enthalpy at pseudo critical temperature with pressure



[A] Pseudo critical temperature [B] Pseudo critical enthalpy

Figure 4 Comparison of calculating results of pseudo critical point

Figure 4 shows the fitting equation has good agreements with the reliable value which is obtained by solving the nonlinear Eq. (4) with iterative method.

$$\left[\frac{\partial c_p}{\partial t}\right]_p = 0 \tag{4}$$

Here the specific isobaric heat capacity is calculated by IAPWS-IF97 property formulations [7].

2.3 Water properties calculation

In ATHLET-SC code, water properties are calculated with the method that combines the look-up table approach and water properties table file for fast calculation of water thermo-physical properties. The data of the water properties table file is calculated by the IAPWS-IF97 property formulations [7]. And the structure of the water properties table file is similar to the stgh2o file of RELAP5 [8], where temperature and pressure are the index variables. There will be two serious problems using this look-up table method: [A] the mutations of the water properties near the critical point will lead to the incorrect data by the above formulation; [B] in ATHLET, a subroutine F(p, h) which returns the single phase properties for a given pressure and enthalpy is needed, but enthalpy has a steep change with temperature near the pseudo critical line, and the subroutine F(p, h) based on the look-up table approach will cause the large errors of water properties near the pseudo critical line (Figure 5).

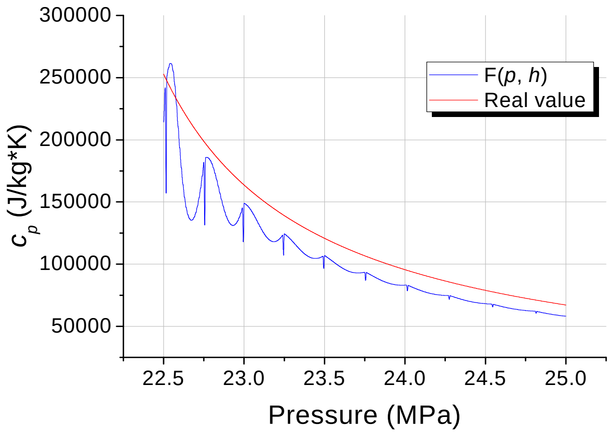


Figure 5 Change of the Specific isobaric heat capacity with pressure
(Enthalpy is fixed, =2200kJ/kg)

In order to ensure the accuracy of water properties near the critical point and pseudo critical temperature, new water properties calculation module is developed and used in place of the look-up table method. Water properties are calculated directly with IAPWS-IF97 formulation in new water properties calculation module. The new module has the following characteristics: [A] water properties near the critical point and pseudo critical temperature have high accuracy; [B] revised the basic equation for high-temperature region 5 of IAPWS-IF97 (as show in Figure 6). For temperatures between 1073K and 2273K, the new equation extends the upper range of validity of IAPWS-IF97 in pressure from 10MPa to 50MPa. ATHLET-SC mod 2 is able to simulate high temperatures phenomenon of SCWR core in specific transient (such as LOCA).

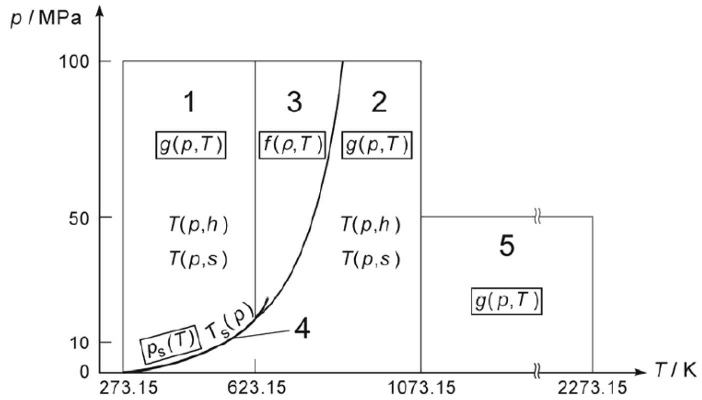


Figure 6 Regions and equations of IAPWS-IF97 [6]

Meanwhile, in order to optimize computed speed, ATHLET-SC mod2 has been modified with two ways as follow: [A] add backward equations [9] [10] for specific volume as functions of v (p, T) and T (p, h) for region 3 of the IAPWS-IF97 to replace the iterative method based on basic equation; [B] improve the data storage structure of water properties for avoiding repeated calls to the properties module.

2.4 Critical flow model

In ATHLET-SC mod2, there is not suitable critical flow model for simulating the discharge mass flow now. The fluid velocity is only limited to the sonic velocity. If fluid velocity exceeds the sonic velocity the momentum equation is switched off from time integration and the fluid mass flow is set equal to the critical mass flow calculation as

$$G_m = w_{son} \times A \times \rho_m \qquad (5)$$

When pressure of fluid is lower than critical pressure (22.064MPa), the fluid sonic velocity is defined as

$$w_{son}^{l} = \left[\left. \frac{\partial \rho^{l}}{\partial p} \right|_{S} \right]^{\frac{1}{2}} \qquad (6)$$

$$w_{son}^{v} = \left[\left. \frac{\partial \rho^{v}}{\partial p} \right|_{S} \right]^{\frac{1}{2}} \qquad (7)$$

$$w_{son} = \left[\frac{1}{\rho_m \left(\frac{1-\alpha}{\rho^{l}} * \frac{1}{\left(w_{son}^{l}\right)^2} + \frac{\alpha}{\rho^{v}} * \frac{1}{\left(w_{son}^{v}\right)^2} \right)} \right]^{\frac{1}{2}} \qquad (8)$$

For 5-equation model, the two fluid mixture sonic velocity is Eq. (8). When pressure of fluid is higher than critical pressure (22.064MPa), the fluid sonic velocity is defined as

$$w_{son}^{sc} = \left[\frac{\partial \rho^{sc}}{\partial p} \bigg|_{S} \right]^{-\frac{1}{2}} \qquad (7)$$

3. Error analysis with the pseudo two-phase method

3.1 Error analysis with the steady-state cases

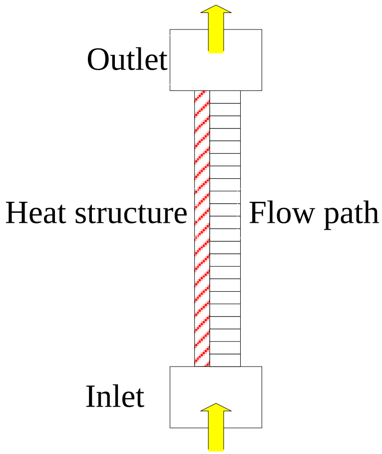


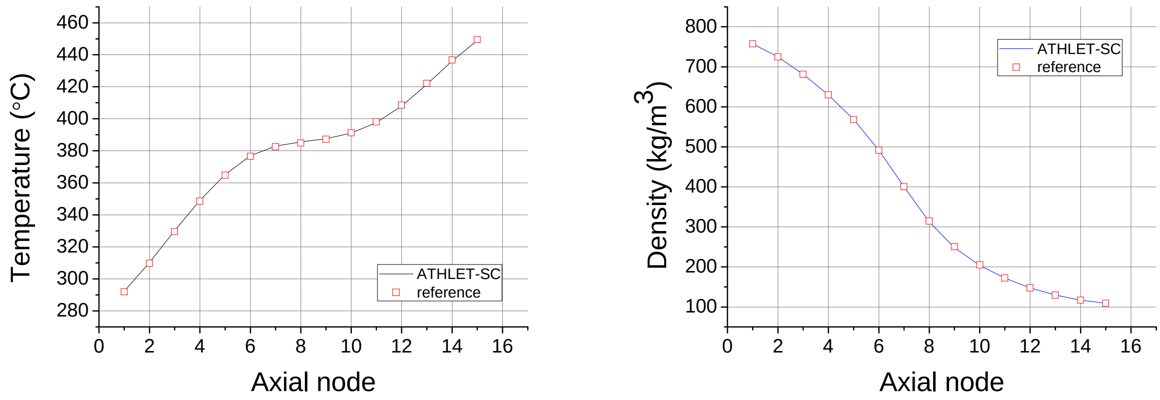
Figure 7 Calculation model

Because of the virtual region of latent heat, the calculation error exists in the pseudo two-phase method for supercritical fluid. The virtual region of latent heat is set at pseudo-critical temperatures. The mutations of the water properties at pseudo-critical temperatures are similar to two-phase transition. And the rate of the mutations decreases as the pressure increases (as show in Figure 2). So the errors of the pseudo two-phase method will increase as the pressure increases. In this paper, the degree of errors under different pressures is studied to determine the feasibility of this new developed two-phase method.

In order to evaluate the errors, several steady-state cases under different pressure are calculated. Figure 7 shows the calculation model of ATHLET-SC code. It is a simplified single channel model consisting of inlet, flow path, heat structure and outlet. And the accurate results (enthalpy, temperature and density distribution in single channel) of these steady-state cases can be obtained with energy balance equation and IAPWS-IF97, and used as reference. So the errors can be evaluated by comparing the results of ATHLET-SC mod2 with the accurate results. The initial conditions for calculation are as follows: system pressures are listed in Table 1; mass flow rate is 100kg/s; inlet temperature is 280℃. The heating power is 172.8MW; and the axial power distribution uses the cosine distribution. The errors of the pseudo two-phase method are summarized in Table 1. The maximum and root-mean-square errors are given for temperature and density. The distribution of temperature and density in Test 3 is presented in Figure 8. Considering the operating pressure of SCWR [10], the highest pressure is set to 29MPa in the tests calculation.

Table 1 Errors of the pseudo two-phase method

		Test1	Test2	Test3	Test4	Test5	Test6	Test7
Outlet pressure(MPa)		23.0	24.0	25.0	26.0	27.0	28.0	29.0
Temperature(℃)	Max error	0.493	0.549	0.698	0.831	1.006	1.019	1.196
	RMS error	0.223	0.340	0.489	0.648	0.797	0.922	1.091
Density(kg/m^3)	Max error	3.165	2.803	2.152	1.997	1.956	1.938	1.928
	RMS error	1.065	0.939	0.799	0.648	0.547	0.532	0.525

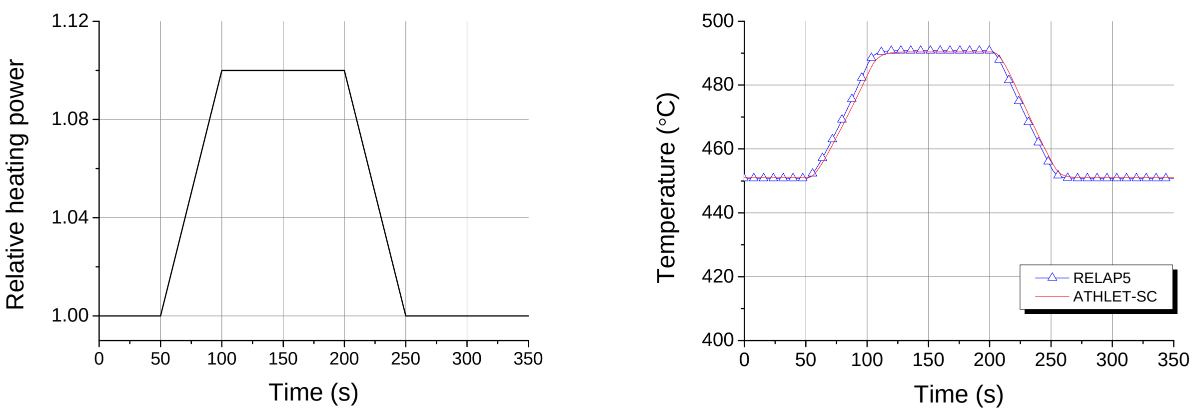


[A] Temperature [B] Density

Figure 8 Main parameter distribution along axial node in Test3

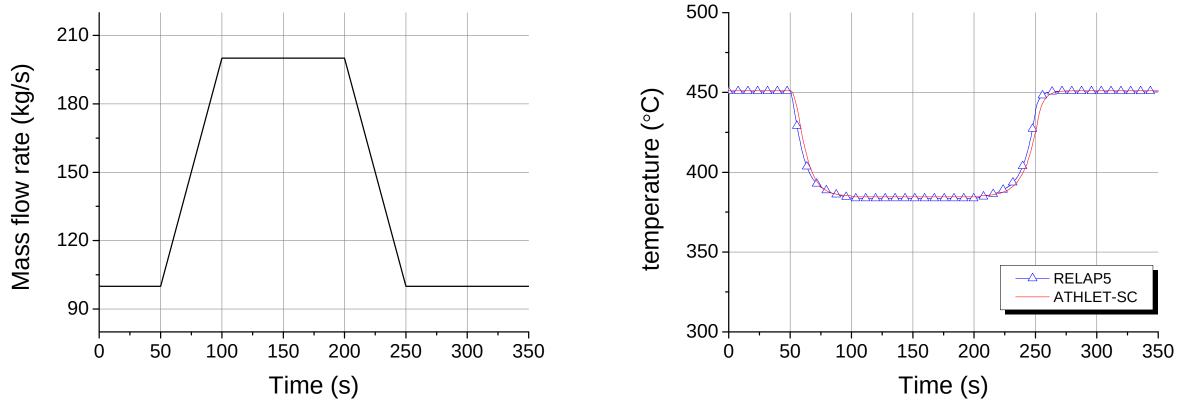
3.2 Error analysis with the transient cases

In this part, RELAP5 is chosen as the reference code for the error analysis of the transient cases. The Single-fluid model is applied in RELAP5 code instead of the two-fluid model. It can be used to simulate the supercritical fluid. So the transient result calculated by RELAP5 code can be used as the reference data for the error analysis of the pseudo two-phase method in dynamic processes. Two transient cases under exactly identical dynamic conditions in sub-critical pressure region are calculated by both the modified ATHLET-SC and the modified RELAP5. Calculation model used here is shown in Fig.7. The initial conditions are as follows: system pressure is 25MPa; mass flow rate is 100kg/s; inlet temperature is 280℃. The initial heating power is 172.8MW. Fig.9 and Fig.10 illustrate the boundary curve and the parameters obtained by the two codes in the calculated samples.



[A] Heating boundary curve [B] Fluid temperature near the outlet

Figure 9 Calculation of transient with heating power changing



[A] Flow boundary curve

[B] Fluid temperature near the outlet

Figure 10 Calculation of transient with mass flow rate changing

The Fig.9 and Fig.10 show that the errors of the pseudo two-phase method in the dynamic calculations are smaller. Combined with the results in table 1, it can be concluded that this pseudo two-phase method is acceptable for supercritical fluid in SCWR analysis.

4. Testing of the Model

4.1 Simulate of the pressurization and depressurization process in single channel

The process of depressurization and depressurization between supercritical and subcritical region can be effectively simulated by ATHLET-SC mod2 code. Changes of main parameters with time at the flow path outlet in the test process are shown in Figure 10. Calculation model imposed in the transients is still the same as in Fig.1. The initial pressure is 25MPa, mass flow rate is 100kg/s, fluid enthalpy is 2080 kJ/kg. And there is no heating power in this test. At the initial condition, a stable flow condition is achieved, and the transient of depressurization starts at 100s. When time goes to 600s the pressure has dropped to 15.0MPa. Then the transient of pressurization starts at 700s. The pressure boundary curve of the test is shown in Figure 11.

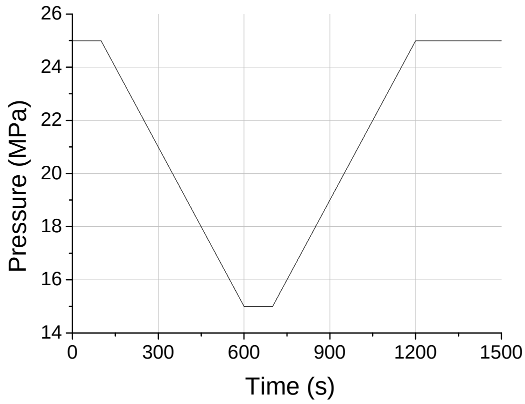
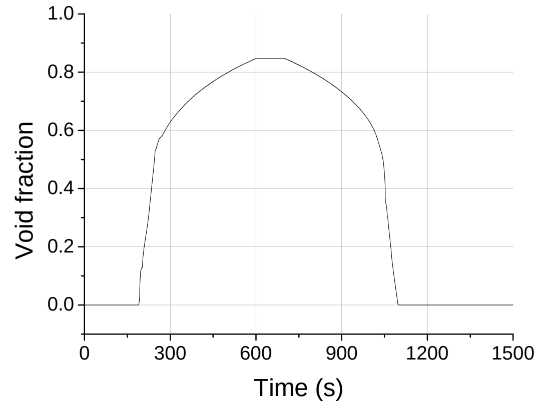
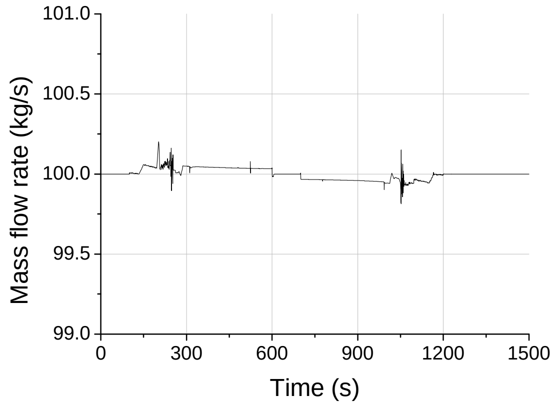


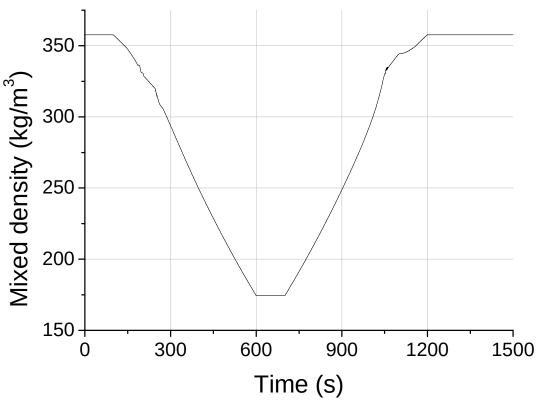
Figure 11 Pressure boundary curve



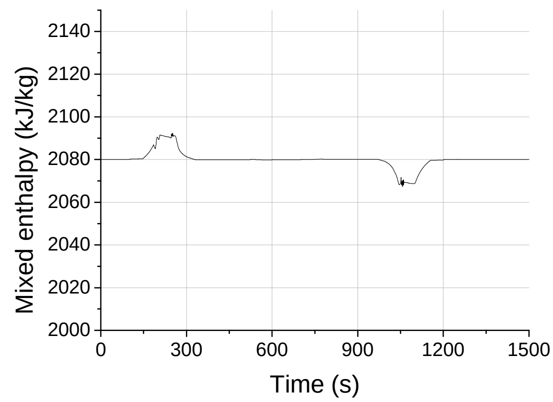
[A] Void fraction



[B] Mass flow rate



[C] Mixed density



[D] Mixed enthalpy

Figure 12 Main parameters with time at the flow path outlet in the test process

Time-behavior of mass flow rate and mixed enthalpy during the test is presented in part B and part D of figures.12. The disturbances of these parameters occur in the trans-critical process. The disturbance of mass flow rate is less than 0.25%. And the disturbance of mixed enthalpy is less than 20kJ/kg. There may be two reasons causing the disturbances: [A] dramatic changes of fluid properties in the trans-critical process caused the numerical instability; [B] the flow instability in supercritical water. Through the principles of the disturbances need the further research based on the experimental data, the width of disturbances is too small to affect the final results of the transients.

4.2 Simulation of the blowdown process

The capability of ATHLET-SC mod2 to calculate the fast transition from the supercritical pressure region to the subcritical pressure region is tested by calculating a simple blowdown accident. The calculation model is shown in figure 13. A straight vertical pipe with 4.0m length and 100mm inner diameter is initially closed and filled with water at state P, T. Then a quick-opening valve is opened at bottom of the pipe within an interval of 0.2s. The volume of the depressurization tank is much larger than the pipe’s. The initial conditions of depressurization tank are as follows: The initial pressure is 1.0MPa; the quality is 1.0. There is no heating power in this experiment. At the initial condition, a stable flow condition is achieved, and the transient of depressurization starts at 5s.

This transient was simulated several times with different initial temperatures, to ensure that ATHLET-SC mod2 can cope with passing through the critical point in which the water property changes are the steepest. The initial temperature are list in Table 2, the initial pressure is constant for all tests.

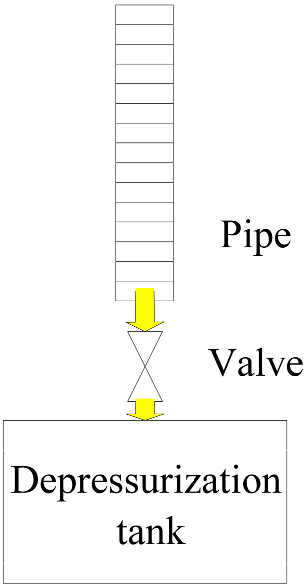
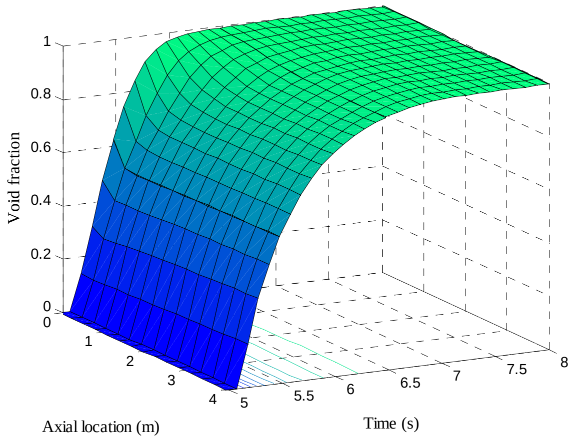


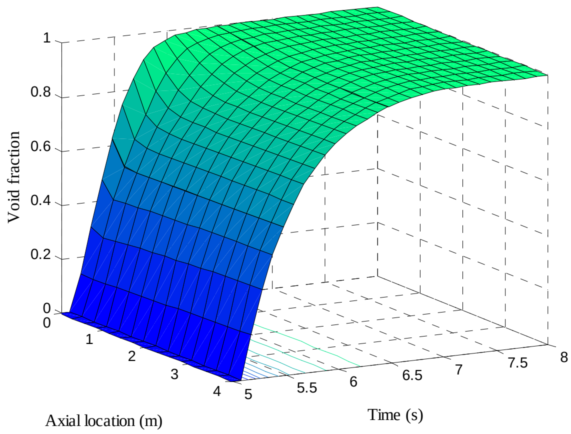
Figure 13 Calculation model

Table 2 Initial conditions of the pipe

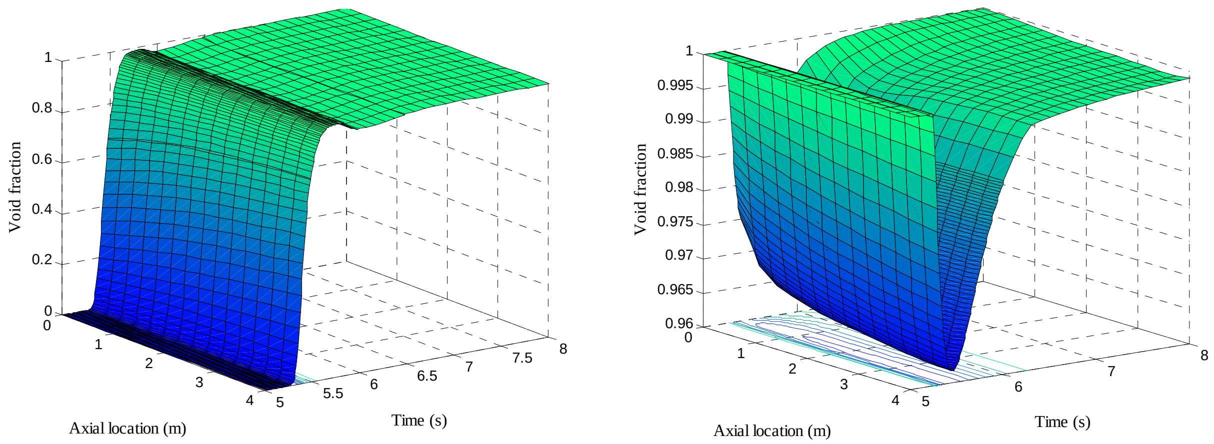
	Test 1	Test 2	Test 3	Test 4
p (MPa)		25.0		
T (℃)	370.0	374.0	383.0	390.0



[A] Test 1

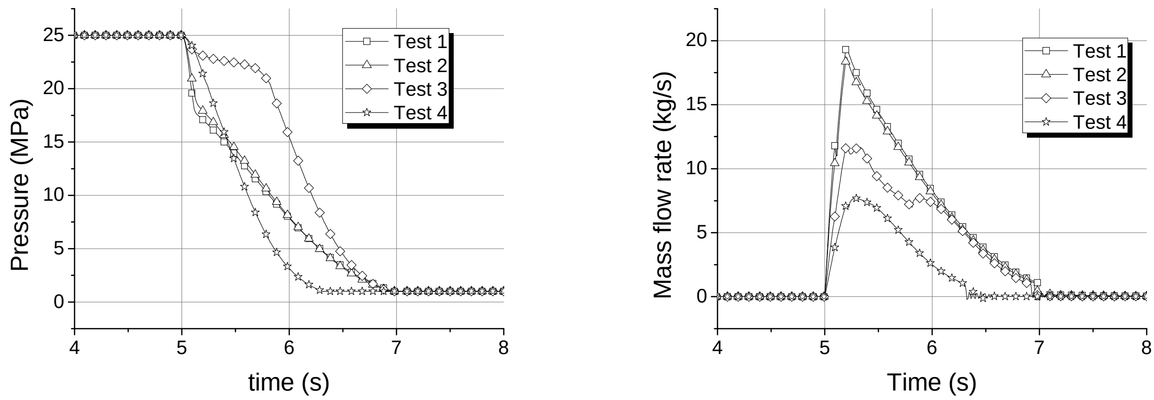


[B] Test 2



[C] Test 3 [D] Test 4

Fig.14 Behavior of void fraction during the blowdown tests



[A] Pressure of pipe [B] Mass flow rate of Valve

Figure 15 Behavior of parameters during the blowdown tests

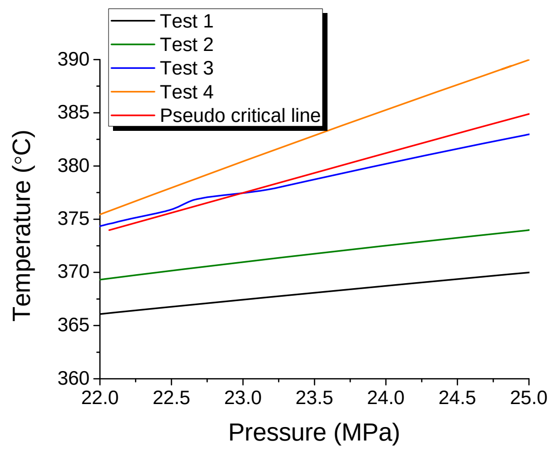


Figure 16 Relationship between temperature and pressure during the blowdown tests (above critical pressure)

Time-behavior of void fraction, pressure and break flow during the tests is presented in Figure 14 and Figure 15. In test 1 and test 2, pressure drops in the pipe very quickly at early stage of the process. This is cause by the low void fraction and the high velocity of sound. Then as the void fraction increased, the fluid mixture density and velocity began to decrease, the value of mass flow rate decreases, and the speed of pressure decrease begins to slow down (Figure 15).

The initial temperature of the test 3 is near the pseudo-critical temperature(≈385℃), and the behavior of temperature during the early process is closed to the pseudo-critical line (Figure 16), sonic velocity of fluid is lower near the pseudo-critical line than other regions (the lowest sonic velocity is at critical point), and density of fluid has a steep change through the pseudo-critical line. This causes a smaller mass flow rate and a slower depressurization than other tests (Figure 15) above the critical pressure. Then, after entering the subcritical pressure region, sonic velocity of fluid raises up, and the rate of pressure drop accelerates.

The initial temperature of the test 4 is higher than the pseudo-critical temperature. So the state of fluid is closed to the gas, and the void fraction of fluid is almost no change in the process. This causes that the behavior of pressure during the test 4 is more stable trend than others. Since the fluid temperature is closed to the pseudo-critical line (Figure 16) and saturation temperature, the energy loss caused by blowdown leads to some temporarily condensation of the fluid (Figure 14-C, D).

Though ATHLET-SC mod2 is capable of calculating the blowdown process from initially supercritical conditions as a conclusion of these tests, critical discharge model of the code is need to develop for more accuracy results of the break flow.

5. Conclusion

In this paper, the system analysis code applicable for SCWR named ATHLET-SC mod2 is modified with pseudo two-phase method on the basis of the ATHLET-SC for simulating the trans-critical transients, which will occur in many operating modes and accidents. The result of error analysis work presents that the pseudo two-phase method for supercritical fluid is acceptable. And some tested calculations and analysis are performed. The results achieved so far verify that the ATHLET-SC mod2 code can be applied successfully to simulate the pressurization and depressurization transient.

Future improving work about ATHLET-SC will focus on modification of the constitutive models (such as critical flow model, wall drag force model) and heat transfer models according to the experimental data. And the LOCA transient of SCWR will be also simulated by the ATHLET-SC mod2 code.

6. Acknowledgment

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Nomenclature

A	Area (m^2)
c_p	Specific isobaric heat capacity (J/kg*K)
G	Total mass flow (kg/s)
h_f^{sup}	Pseudo-saturation enthalpy of liquid in supercritical pressure (kJ/kg)
h_g^{sup}	Pseudo-saturation enthalpy of gas in supercritical pressure (kJ/kg)
$h_{p\text{-}critical}$	Pseudo-critical enthalpy (kJ/kg)
h_{fg}^*	Enthalpy of vaporization (kJ/kg)
p	Pressure (MPa)
S	Entropy (kJ/kg*K)
T	Temperature (K)

w_{son} Sonic velocity (m/s)
α Void fraction
ρ Density (kg/m^3)

Subscripts

l Liquid
v Vaper
sc Subcritical pressure region
m Mixture

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