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A NUMERICAL SIMULATION OF POOL BOILING USING CAS MODEL

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ABSTRACT

This paper presents a new numerical model, called the CAS model, for boiling heat transfer. The CAS model is based on the cellular automata technique that is integrated into the popular–SIMPLER algorithm for CFD problems. In the model, the cellular automata technique deals with the microscopic non-linear dynamic interactions of bubbles while the traditional CFD algorithm is used to determine macroscopic system parameters such as pressure and temperature. The popular SIMPLER algorithm is employed for the CFD treatment. The model is then employed to simulate a pool boiling process. The computational results show that the CAS model can reproduce most of the basic features of boiling and capture the fundamental characteristics of boiling phenomena. The heat transfer coefficient predicted by the CAS model is in excellent agreement with the experimental data and existing empirical correlations.

Keywords: numerical simulation, pool boiling, SIMPLER, cell automata, CAS model.

INTRODUCTION

Pool boiling is often encountered and widely used in the manufacturing, power and chemical industries because of its high efficiency of heat transfer. It is essential to have ability to predict accurately the rate of heat transfer in pool boiling under various pressures and geometry conditions so that one can design the heat transfer equipment with reduced cost, size or weight.

Great efforts have been devoted to measurements and modeling of boiling process in the past several decades. Various correlations have been developed to calculate pool boiling heat transfer. Nevertheless, the physical mechanism of pool boiling is still not fully understood. The majorities of the correlations available are empirical and can only be applied in relatively narrow ranges with considerable error bands.

Through the years, researchers are seeking for valid numerical methods to simulate the pool boiling process. Many models have been proposed and can be divided into two major categories: the deterministic models and probabilistic models. The deterministic models include the models using the traditional CFD methods (finite difference or finite element) to solve the conservation equations of mass, momentum, and energy, so as to determine the motion, interaction, and thermodynamic variations of the system. Once the governing equations, boundary and initial conditions are given, the results will be obtained in a deterministic way. For example, Wang *et al.* [1] put forward a model that takes into account the time development of boiling phenomena in both micro- and macro-scales. In micro-scale the model includes a detailed description of instantaneous local conduction, convection, energy and mass exchanges across the interfaces. The macroscopic descriptions of the model are then emerged as a natural consequence in a deterministic way by keeping track of the microscopic boiling dynamics. Similarly, He *et al.* [2] proposed a model based on the numerical macrolayer method. The boiling curves were reproduced numerically by determining the macrolayer thickness. It postulated that vapor stems were formed on the active cavity sites with a certain contact angle and the evaporation occurs at the liquid-vapor interface. An initial spatial pattern of vapor stems was assumed and the experimental macrolayer thickness with wall superheat was employed. Subsequently, the heat flux was calculated according to the model and the simulated boiling curves were obtained.

The deterministic models discussed above are based on the solutions of the partial or differential equations of continuous system. The probabilistic models, on the other hand, deal with microscopic dynamics based on the evolving rules for temporal and spatial discrete systems. The complex behaviors of the whole system can be described by simple interactions of local regions in the probabilistic models, and the macroscopic physical characteristics can then be obtained by statistic average of microscopic variables. Many approaches have been tried to develop a probabilistic model. For example, Yang *et al.* [3] have developed a model that is based on the lattice-Boltzmann method. The model describes the hydrodynamic aspects of bubble coalescence under nucleate boiling condition by simulating the growth and detachment behavior of multiple

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bubbles generated on the horizontal, vertical, and inclined downward-facing surfaces. Kimura [4, 5], on the other hand, has employed a molecular dynamics method to simulate the heterogeneous nucleation of liquid droplets on a solid surface. The spherical automata model [6] and the coupled map lattice method (CML) [7] have also been attempted for simulation of boiling.

In reality, boiling is a complex nonlinear dynamic process. First, the nature of a boiling process is largely determined by its microscopic aspects, e.g. embryo nucleation and surface roughness. The microscopic effects eventually exhibit in a macroscopic manner. Second, the boiling process seems to be stochastic without any rules to be abided by; no one can predict precisely where or when the next bubble will generate, vanish or coalesce. However, once the initial conditions and boundary conditions are given, the macroscopic boiling phenomenon emerges at the time as expected as if it has been planned in advance, in other word, boiling seems also to be deterministic. Third, the boiling field is filled with a large amount of bubbles generated with the vapor-liquid interface kept on moving. As a whole, however, it is still a continuous system. Therefore, boiling is a process unifying the deterministic and stochastic, discrete and continuous, microscopic and macroscopic aspects. The existing models, either deterministic or probabilistic, are not able to capture the fundamental nature of the boiling process. The deterministic models neglect the random factors and phenomena occurred in microscopic level such as coalescence and vanishing of bubbles as well as the surface roughness effect of the heater. On the other hand, the probabilistic models have advantages over the traditional deterministic models in simulating random boiling phenomenon but it brings indelible statistic white noises to the macroscopic statistics.

This study proposes a new model, namely CAS model, for theoretical simulation of a boiling process. The CAS model integrates the nonlinear method - Cellular Automata [8] - with the traditional CFD method-SIMPLER (Semi-Implicit Method for Pressure Linked Equations Revised) [9]. The paper presents a detailed description of the model. Testing results will be also presented to demonstrate the feasibility and effectiveness of the CAS model in simulating the boiling phenomena.

NOMENCLATURE

c_p	specific heat
g	gravity acceleration constant
h	enthalpy
h_{fg}	latent heat of evaporation
p	pressure
P	number defined in Eq. (6)
r	radius
Ra	surface roughness
S	source terms
t	time
T	absolute temperature
T_{sat}	saturation temperature
u	velocity along x coordinate
v	velocity along y coordinate
x	random number, defined in Eq. (6)

Greeks

ρ	density
σ	surface tension
μ	kinematic viscosity
k	thermal conductivity

Subscripts

e	equilibrium
i	index number
ran	random number
cut	cut-off value

Superscripts

L	liquid
V	vapor

THE CAS MODEL

In pool boiling, a growing bubble causes the drop of the surface temperature adjacent to it. The bubbles also influence each other due to heat absorption or release as the neighbor vapor bubbles generate, grow and vanish. It's such continuous competition and cooperation that determines the boiling heat transfer. Such a nonlinear interaction is very difficult to be simulated by using a traditional, deterministic CFD method. Therefore, the Cellular Automata technique is introduced in the CAS model to simulate such nonlinear interactions among bubbles in a boiling process. The Cellular Automata (CA) method alone, however, cannot completely describe the boiling process because of the existence of white noises coming from its statistical nature. Therefore, it is proposed here that the cellular automata technique is incorporated into a traditional CFD algorithm, with the cellular automata method dealing with the microscopic non-linear dynamic interactions of bubbles while the traditional CFD algorithm is used to determine the macroscopic parameters, such as pressure, temperature. Here, Patankar's SIMPLER method [9] is employed for the CFD treatment.

Cellular Automata deals with arrays of discrete cells with discrete values. The value at each cell evolves deterministically with time according to a set of definite rules involving the values of its nearest neighbors.

Cell and Grid

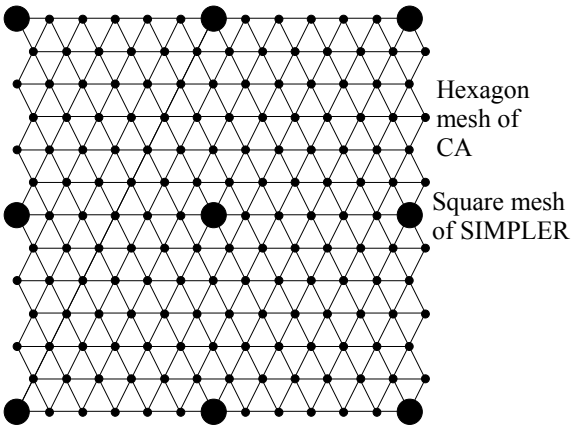


Figure 1. Two superposed grid schemes used in the CAS model: a hexagon mesh for CA and a square mesh for SIMPLER algorithm.

In the present CAS model, the computational domain is divided into regular hexagon cell lattice of equal size (in two

dimensions), and a SIMPLER square mesh is then superimposed to the cellular automata network as shown in Fig.1. The regular mesh of the hexagon cells with a much finer scale is used for modeling of vapor bubble formation with the CA technique. Each cell is characterized by different variables (e.g., temperature, orientation) and states (liquid or vapor). The aim of this combination is in order to predict simultaneously the microstructure development as a function of the thermal field and the influence of the latent heat release of the cells on the calculated thermal history.

Governing Equations

Though boiling phenomena is complicated, the thermal convection and diffusion is still governed by the equations of motion (Navier-Stokes equations) and the equation of energy conservation.

Mass conservation equation:

$$\frac{\partial \rho}{\partial t}+\frac{\partial (\rho u)}{\partial x}+\frac{\partial (\rho v)}{\partial y}=0 \tag{1}$$

Momentum conservation equation-x:

$$\frac{\partial (\rho u^2)}{\partial x}+\frac{\partial (\rho uv)}{\partial y}=-\frac{\partial p}{\partial x}+\frac{\partial}{\partial x}\left(\mu \frac{\partial u}{\partial x}\right)+\frac{\partial}{\partial y}\left(\mu \frac{\partial u}{\partial y}\right) \tag{2}$$

Momentum conservation equation-y:

$$\frac{\partial (\rho uv)}{\partial x}+\frac{\partial (\rho v^2)}{\partial y}=-\frac{\partial p}{\partial y}+\frac{\partial}{\partial x}\left(\mu \frac{\partial v}{\partial x}\right)+\frac{\partial}{\partial y}\left(\mu \frac{\partial v}{\partial y}\right)-g\rho \tag{3}$$

Energy conservation equation

$$\frac{\partial (\rho h)}{\partial x}+\frac{\partial (\rho h)}{\partial y}=\frac{\partial}{\partial x}\left(k \frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(k \frac{\partial T}{\partial y}\right)+S \tag{4}$$

The meanings of symbols are defined in the nomenclature.

Treatment of Bubble Nucleation

During nucleate boiling, steam bubbles are generated from specific sites which are cavities or scratches on the surface that can trap vapor. The total number of active sites available depends on the surface condition, material and the heat flux level. In the CAS model, bubble nucleation is randomly initiated on the surface after the cell temperature satisfies the following nucleation discriminant [10]:

$$T^L - T_{sat} > \frac{2\sigma T_{sat}}{\rho^V h_{fg} r_e} \tag{5}$$

where T^L is the liquid temperature, T_{sat} is the saturation temperature, σ is the surface tension, ρ^V is the density of vapor, h_{fg} is the latent heat, and r_e is the critical radius of bubble nucleus.

Bubble nucleation in boiling is treated as a random process in the CAS model through a random number, x_{ran}, that is generated following the following Poisson distribution function:

$$P(Ra, x_{ran}) = \frac{e^{-f(Ra)} f(Ra)^{x_{ran}}}{(x_{ran})!} \tag{6}$$

where Ra is the arithmetic roughness of the surface. The expression $f(Ra)$ in Eq. (6) is determined by the material of heater surface and the liquid. For each cell on the surface and any given x_{ran} and Ra, Eq. (6) calculate a number P. Once P is larger than a prescribed cut-off value P_{cut}, this surface cell (or cite) is then nucleated with vapor bubble. The cell then converts to active nucleus from which steam bubble grows.

Rules of Cell Evolution

In the CAS model, the cells of Cellular Automata have values of either zero or one. At each time step, all of the sites of the domain are simultaneously updated by applying rules to the neighborhoods of each site. The rules of cell evolution are defined as follows:

- Any cell with its three nearest neighbor cells vaporized stays vaporized.
- A vaporized cell with two nearest neighbor cells vaporized remains vaporized.
- All other cells remain as a liquid state.
- During the growth of a vapor bubble, the cells that were caught by the growing bubble become active nucleuses.
- When a growing cell has all of its neighbors with a non-zero index number, it will be no longer incremental.

Coupling of the CA model with the SIMPLER Algorithm

The coupling of the Cellular Automata with the SIMPLER algorithm is realized through the energy conservation equation, Eq. (4). It is known that the enthalpy variation of a control volume in a boiling process consists of two parts: one is caused by the variation of temperature (sensible heat); another is caused by the phase transition (latent heat). Therefore, the variation in the enthalpy of any given node n (δh_n) can be calculated based on the temperature variation (δT_n) of the node and the variation of the void fraction (δv_n) of the node :

$$\delta h_n = \rho c_p \delta T_n - h_{fg} \delta v_n \;= \rho c_p \left[T_n^{t+\delta t} - T_n^t \right] - h_{fg} \delta v_n \tag{7}$$

The variation of the nodal temperature and enthalpy are obtained by solving the energy conservation equation together with all other governing equations based on the SIMPLER algorithm. The temperature at each cell is then determined by linear interpolation using the nodal temperatures obtained. For example, the temperature of the cell i at time t, T_i^t, can be obtained by the bi-linear interpolation from the temperatures of the four nodal points of the SIMPLER square meshes around T_n^t:

$$T_i^t = \sum_n c_{i,n} \cdot T_n^t \tag{8}$$

where $c_{i,n}$ are the interpolation coefficients.

The state of each cell is determined by the method described in the section "Treatment of Bubble Nucleation" and evolves according to the rules listed in the section "Rules of Cell Evolution". When the state of a cell is changed from liquid to vapor, the void fraction variation at this cell is expressed as δv_i. The void fraction variation of the associated nodal point n, δv_n, is then calculated by that of all the cells associated with it:

$$\delta v_n = \frac{\sum_i c_{i,n} \delta v_i}{\sum_i c_{i,n}} . \tag{9}$$

Once δv_n is determined, the nodal temperature can then be updated based on Eq. (7):

$$T_n^{t+\delta t} = \frac{\delta h_n + h_{fg} \delta v_n}{\rho c_p} + T_n^t . \tag{10}$$

Calculation Procedure

Figure 2 shows the flow chart of the CSA model. At the beginning of the simulation, each cell is given the same initial temperature below the liquidus, and assigned a state index

equal to zero. The sites located immediately next to the wall have a reference number which indicates that they belong to this boundary. The time-matching calculation is then started. Periodic boundary condition is assumed at both sides of the boiling field. Therefore, the cells on the right boundary have their east neighbor located on the left boundary and vice versa.

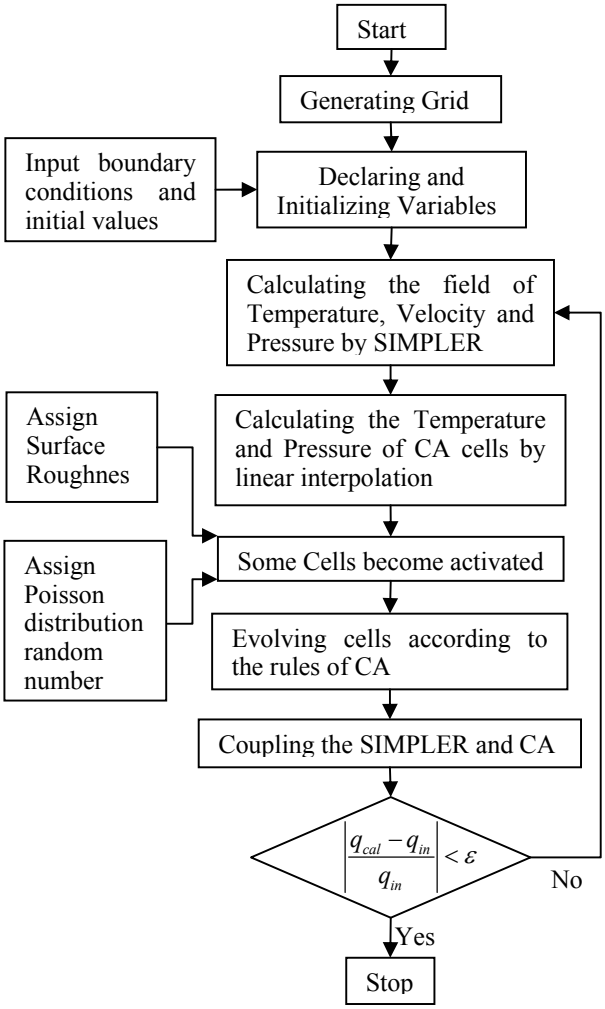


Figure 2. Flow chart of the CAS model.

EXPERIMENTAL APARATUS

The boiling vessel is made of stainless steel with 110×110 mm^2 cross section and 130 mm height (shown in Fig. 3). The heating surface is made of a quartz glass plate with 20×60 mm^2 area (4 mm in thickness) and exposed to the test liquid directly. On the surface opposite to the heat transfer side, a transparent ITO film is coated and operated as heater by applying electric current through it. On the heat transfer side, thin copper and constantan electrodes of 1.2 μm thicknesses are coated directly on the glass substrate, see Fig. 4. Two electrodes were made contact at the end of each as the hot conjunction to form a thermocouple for temperature measurement. Total nine thermocouples were employed. The power input is determined from the measured electric voltage and current imposed on the heater. The system pressure is maintained constant at 1 atm by a condenser connected with the boiling chamber.

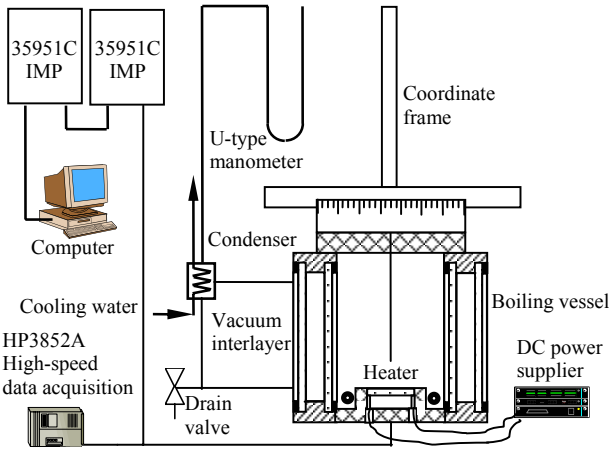


Figure 3. A schematic of the boiling vessel and instrumentation.

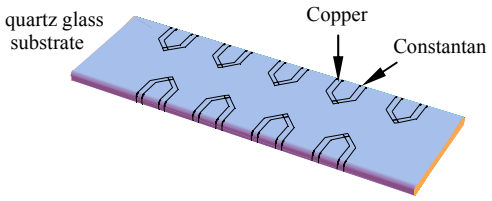


Figure 4. A schematic of the heater (on the back) and the thermocouple distribution.

RESULTS AND DISCUSSION

The CAS model has been employed to predict pool boiling of water under various conditions. The model predictions are compared with available experimental data. The initial temperature of water ranges from 30℃ to 100℃, *i.e.*, from a subcooled to a saturated condition. A two-dimensional square is chosen as the boiling field of calculation for the convenience. The bottom of the square is heater with a constant heat flux and the temperature at the top of the field is fixed at a constant prescribed temperature. A periodic boundary condition is applied to both sides of the boiling field.

Boiling Curve

Figure 5 shows a comparison of the boiling curve predicted by the CAS model (solid line) with the experimental data. For comparison, Figure 5 also include the predictions from the two empirical correlations proposed by Михеев[10] and Rohsenow[11], respectively. It is found that the CAS model prediction is in an excellent agreement with both the experimental data and the empirical correlations, in particular in the high superheat region. In the low superheat region, the CAS model a little underestimates the heat flux. A good agreement between the model and the data in the high superheat region indicates that the present CAS model captures

the fundamental nature of boiling when vapor bubbles are abundantly generated and frequently interacted.

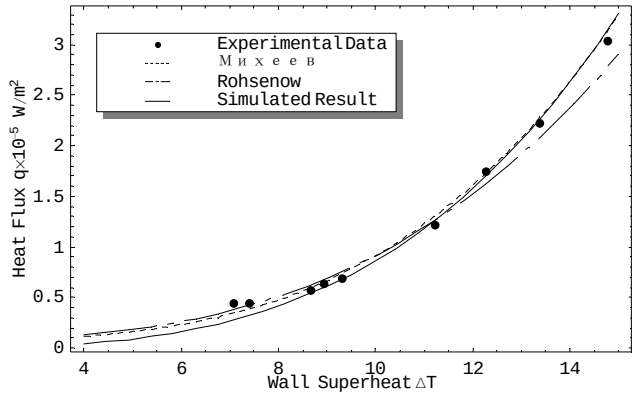
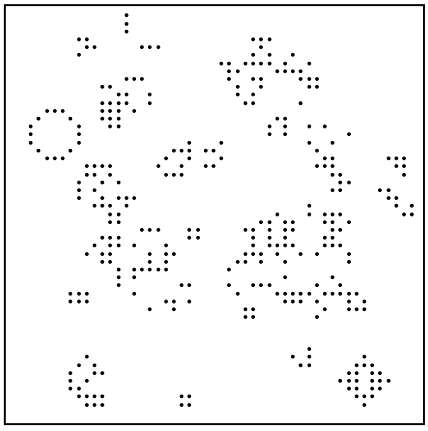
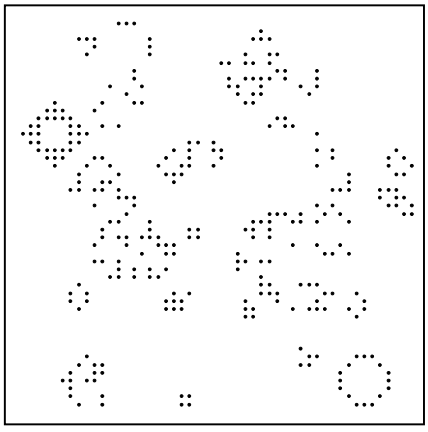


Figure 5. Comparison of the CAS model prediction with experimental data and the empirical correlations.

Snapshots of the Boiling Pattern



(a)



(b)

Figure 6. Two snapshots of the pool boiling pattern.

The snapshots of boiling pattern are given in Figure 6. The state of boiling is changing continuously according to the evolving rules of the CAS model at each time step. Each state is recorded as a frame of a "video". Herein, only two snapshots of them are chosen arbitrarily for demonstration purpose. By playing these frames one after another, one can visualize the entire boiling process with major boiling modes, including nucleation, growth, coalescence and condensation of vapor bubbles.

Effect of the Surface Roughness

Figure 7 shows the predicted boiling curves for two surface conditions: a rough surface (*Ra*=14.27) and a smooth surface (*Ra*=9.38). As one can see, the rough surface produces a higher heat flux than that of a smooth surface, due to increased surface active sites. The present CAS model is able to reproduce the roughness effect, at least in a qualitative way.

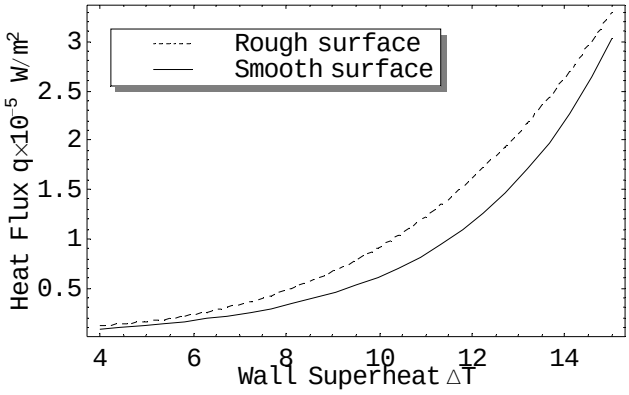


Figure 7. Predicted boiling curves for two surfaces with different surface roughness.

CONCLUSION

The paper presents a new model for pool boiling. The model integrates the cellular automata method into a traditional CFD algorithm. Computational experiments demonstrate that the CAS model is able to capture the essential physics underlying pool boiling and its prediction agrees well with our own experimental data as well as the empirical correlations available in the literature.

The study demonstrates that the cellular automata technique is compatible with the traditional CFD method. Since the CAS model can be considered as an approach coupling microscopic molecular dynamics and conventional macroscopic fluid dynamics, it should be also applicable in the cases where the microscopic statistics and macroscopic description of a system are all considerably important, e.g., the multiphase multi-component systems involving surface tension, capillarity and phase transition.

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