Final Technical Report

on the U.S. Department of Energy Phase I SBIR Project

A New Computational Tool for Simulation of 3-D Flow and Heat Transfer in Boiling Water Reactors

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This Phase I work has developed a novel hybrid LBM model for the simulation of non-ideal fluid thermodynamics, and demonstrated that this model can be used to simulate fundamental two-phase flow processes including boiling initiation, bubble formation and coalescence, and flow-regime formation. All the technical objectives of Phase I have been met successfully. Below we review the main developments and accomplishments of Phase I.

Section 1. Formulation of multiphase lattice Boltzmann algorithm with thermodynamics

As described in the Phase I proposal, the lattice Boltzmann method has been shown to be ideally suitable for the simulation of flows involving multiple immiscible phases, such as a water/vapor mixture [24]. On the other hand, the crucial missing piece in all previously existing developments is that they are only applicable for isothermal flow situations, since no technique for dynamic coupling of temperature with the multiphase lattice Boltzmann algorithm existed in the published literature [22]. In other words, the temperature field in the models used before this Phase I effort was undertaken has been represented either as a prescribed constant or, at best, having some prescribed gradient values. The fundamental reasons for these simplifications are: 1) lattice Boltzmann models involving temperature dynamics based on a self-consistently generated energy degree of freedom are known to be highly unstable numerically [21,28]. The computational cost required to overcome this problem is extremely high in practice [23,25], and 2) for simulations involving non-ideal gas equations of state, non-local interactions, which introduce additional computational and numerical stability problems, are essential. These

simplifying assumptions make it impossible to track the energy transport and conservation that are required to simulate the temperature dynamics needed to describe the water/vapor mixture flow typical for BWR applications. In Phase I we have successfully addressed and overcome the two LBM limitations described above. We developed a novel LBM approach that allows for simulation of multiphase, non-ideal fluid thermodynamics. This model includes terms that describe the non-local interactions, allowing the simulation of non-ideal fluids. It describes the fluid thermodynamics by modeling the multiphase density and fluid velocity evolution via the lattice Boltzmann method, while the temperature dynamics is computed by solving a scalar transport energy equation.

Implementation of lattice Boltzmann algorithm with non-ideal gas equation of state

We have implemented a lattice Boltzmann algorithm that simulates non-ideal gas fluid flow. This approach has demonstrated its ability for capturing the intrinsic phase separation physics in boiling processes involving a mixture of water and vapor. The basic lattice Boltzmann equation is given as

$$f_i(x + c_i, t + 1) - f_i(x, t) = C_i(x, t) + \delta f_i \quad (1)$$

where the collision term $C_i(x, t)$ is the so called BGK model that determines the viscosity in terms of the relaxation time,

$$C = -\frac{1}{\tau}(f - f^{eq}) \quad (2)$$

Without the additional term δf_i the momentum moment of lattice Boltzmann models of this kind gives rise to the Navier-Stokes fluid flow equations [19,20]:

$$\begin{aligned}\partial_t \rho + \nabla \cdot (\rho \vec{u}) &= 0 \\ \rho(\partial_t \vec{u} + \vec{u} \cdot \nabla \vec{u}) &= -\nabla p + \nabla \cdot (\rho \nu \nabla \vec{u})\end{aligned}\tag{3}$$

where $\rho, \vec{u}$ are, respectively, the fluid density and velocity. The pressure p obeys an ideal gas like equation of state, $p = RT_0 \rho$, where T_0 is a prescribed temperature value, and R is the universal gas constant. The resulting kinematic viscosity is determined by the relaxation parameter, τ , as $\nu = (\tau - 1/2)T_0$.

One of the key developments of our Phase I work was to use the additional term δf_i in equation (1) in order to produce desired non-ideal gas properties. Generally speaking, this additional term represents a body-force. The first key observation is that a non-ideal gas equation of state is produced if this body force term is self-consistently generated from the gradient of the local density and temperature values. Specifically, the momentum due to the additional term (δf_i) in (1) is explicitly constructed such that:

$$\sum_i c_i \delta f_i = -\nabla p(\rho, T) + \nabla(R\rho T_0)\tag{4}$$

Here $p(\rho, T)$ can be in principle any arbitrary function of local density and temperature, for example the one corresponding to the classical Van der Waals equation of state or a more realistic one. The second term in (4) is used to cancel the existing ideal gas pressure in the

original lattice model. As a consequence, an algorithm describing the thermodynamics of a fluid with a non-ideal gas equation of state is obtained when the evolution of the temperature distribution or an energy equation is provided.

Figure 1 shows a set of graphs describing fluid density distributions at different times in a square domain resembling a cross-section of a BWR fuel assembly. Spontaneous phase separation between water and vapor phases is predicted by the new Lattice Boltzmann code developed in Phase I. Vapor bubbles (light shade) and water (dark shade) emerge out of the initial two-phase mixture as a result of infinitesimally small random density fluctuations. In time, the small vapor bubbles coalesce into ever larger size bubbles which directly describes the expected behavior of realistic fluid undergoing phase transition. To demonstrate the physics of this process, we used the Van der Waals non-ideal gas equation of state. In this case, pressure is related to the local specific volume V (i.e. the inverse number density $V = 1/\rho$) and temperature T according to

$$(p + \frac{a}{V^2})(V - b) = RT \quad (5)$$

where a and b are constant parameters which depend on the fluid being analyzed. This choice of the equation of state, although a simplification of reality, has the advantage of having a simple analytical form. In addition, the Van der Waals equation of state (EOS) is the most familiar non-ideal gas EOS and its thermodynamic properties are well understood and defined [26]. This makes it suitable for demonstrating the fundamental capability of the current approach for multiphase flow simulations.

We have shown during Phase I that the key physical features of spontaneous phase separation in our algorithm do not depend critically upon peculiarities of the equation of state (EOS), as long

as it is non-ideal. Figure 2 plots pressure (p) and specific volume (V) relations (isotherms) at three representative temperature (T) values according to Eq.(5). The key difference between a fluid with a non-ideal gas EOS (such as Van der Waals, shown in Figure 2 and an ideal gas is that the former exhibits phase separation under certain conditions. Namely, at low enough temperature, the pressure of such a fluid is no longer a monotonically decreasing function of the specific volume so that a given pressure corresponds to more than one density value.

Consequently, a substance with an initial intermediate density will undergo a spontaneous phase separation into two immiscible phases. As shown in Figure 2, the resulting density values at a given temperature are located at the intersections of a given pressure isotherm (a solid line with symbols) and the phase coexistence curve (the thick solid line). This fundamental physical mechanism is robust across a wide range of equations of state and when implemented in the algorithm developed during our Phase I research realistically describes formation of multiple phases typical of water/vapor mixture. The critical point values for the Van der Waals fluid are completely determined by the constant fluid-dependent parameters a and b : $V_c = 3b$,

$T_c = \frac{8a}{27bR}$, $p_c = \frac{a}{27b^2}$. Also in Figure 2, we insert an isotherm of the water/vapor equation of

state obtained from an experimental table.

Fig 1a.

Fig 1b.

Fig 1c.

Figure 1. Spontaneous water/vapor phase separation process calculated using the new Lattice Boltzmann code. Three consecutive times are shown.

This has been verified in the current algorithm. The results shown in Figure 1 are obtained for $T = 0.9T_c$ and ρ chosen to be within the phase co-existence domain. As mentioned before, tests using alternative equations of state yield similar results.

Figure 2.

Implementation of a scalar solver for the temperature dynamics

As discussed above, a non-trivial thermal multiphase flow requires specification of the temperature dynamics. For this purpose, during Phase I we have developed and incorporated in the new LBM model a finite difference scheme for the solution of the energy equation, which describes the scalar transport of energy in multiphase flow. We have completed the basic software protocol of the new hybrid approach by coupling this scalar energy equation to the

above multiphase lattice Boltzmann algorithm. The specific form of the energy equation used currently is the fluid internal energy e ,

$$\rho(\partial_t e + \vec{u} \cdot \nabla e) = -p \nabla \cdot \vec{u} + \nabla \cdot \left(\rho \frac{\kappa}{c_v} \nabla e \right) \quad (6)$$

This in turn determines the temperature via $e = c_v T$, once the heat capacity c_v is specified. The first term on the right hand side of (6) includes some effects of the latent heat, so that the temperature drops when water vaporizes as a result of $\nabla \cdot \vec{u} > 0$. Equation (6) is exact as long as the heat capacity (specific heat), the pressure behavior at the interface between the two phases, as well as the thermal conductivity κ are specified. An alternative formulation which has also been explored but not implemented in Phase I involves the enthalpy equation,

$$\rho(\partial_t h + \vec{u} \cdot \nabla h) = (\partial_t p + \vec{u} \cdot \nabla p) + \nabla \cdot \left(\rho \frac{\kappa}{c_p} \nabla h \right) \quad (7)$$

One motivation for this alternative is that, unlike the first term on the right hand side of (6) which is highly discontinuous across interfaces due to density jumps, the pressure distribution (and its functional dependencies) is continuous. A smoother quantity is always more desirable to deal with numerically. Furthermore, the enthalpy equation in the above differential form more accurately describes the physics of multiphase flows than the internal energy equation.

However, the enthalpy equation requires more careful consideration with respect to the treatment of the pressure time derivatives.

In Phase I we conducted extensive study and testing of numerical schemes for numerical solution of these generalized energy equations in the context of multiphase flow. The best candidate

proved to be the extended Lax-Wandroff 2nd order finite difference scheme that has been formulated and implemented in the final software versions [27]. The high accuracy and stability of this method is illustrated in the simulation with the geometry presented in Figures 3-4. The results are presented in detail in Section 3.

Section 2. Implementation of the software protocol

The fundamental algorithm formulated above has been implemented on several computational platforms. In order to simulate non-trivial flow scenarios relevant to boiling water reactor applications, a wide range of boundary condition physics has been investigated and algorithmically developed. These include three essential ingredients:

- 1) Inlet and outlet conditions: As proven by numerous tests, appropriate boundary conditions are crucial for faithful simulation of multiphase flows. Keeping in mind of BWR applications, we have experimented with various conditions for channel flows. We found it to be most desirable to use for the inlet the specified velocity, density, and temperature boundary condition, while the outlet is based on free flow conditions and consistent with the overall mass flux conservation. The particular boundary conditions that have been successfully used in this Phase I research is to apply outlet boundary conditions corresponding to zero normal derivatives of both density and temperature, while specifying the fluid velocity according to the mass flux value at the inlet.

- 2) Thermal boundary conditions at the solid surface: In order to simulate thermal walls, we have developed an algorithm for heat transfer at the wall that either can specify a heat flux or a prescribed wall temperature. This algorithm is shown to be stable and capable of handling arbitrary geometries and shapes. (Figures 3-4) This is important for BWR applications involving realistic reactor geometries/setups.

- 3) Boundary conditions for multiphase lattice Boltzmann solver at a solid surface: This algorithm includes two parts. First we have implemented the no-slip condition on the solid surface in the lattice Boltzmann solver. Essentially, this condition is achieved via the so called ``bounce-back'' of particles on the solid walls. Indeed, this approach gives a 2nd order accurate realization of the no-slip condition [13,14]. Secondly, we have implemented an algorithm which can control the surface wetting properties. Although this effort was originally planned for Phase II we have discovered early in this research that it is not only feasible but actually helpful for successful accomplishment of Phase I. The reason is that the degree of wetting of water phase at the boundary makes a real difference even for relatively simple multiphase channel flows. If the surface is wetting for water, then vapor bubbles are more likely to detach from the surface and water is more likely to layer along the solid surface. Consequently, we have discovered that the resulting heating rate of the flow is strongly affected by the choice of the wetting property. In addition to these essential processes on the wall, we also have developed and implemented an algorithm for simulating seeds of vapor nuclei via imposing certain random density fluctuation near wall. This allows for significantly enhanced vaporization at the heated solid surface, similar to what is happening in reality.

Section 3. Simulation results and validation of fundamental physics

The software protocol described above has allowed us to perform a series of simulations of prototype BWR multiphase flow with the goal of validating the fundamental physics and the numerical implementation. The essential results consist of two parts: 1) simulations of single phase thermal flows in complex geometries, and 2) demonstration of two phase thermo-hydrodynamics fundamental capabilities in a 2-D channel flow.

Prototype Nuclear Reactor Simulations

As described above, we have developed and implemented a scalar transport solver for dynamic temperature evolution, together with the implementation of the corresponding boundary condition schemes allowing for simulation of flows in a BWR fuel bundle. The domain used in this simulation represents the lower 40% of the actual fuel bundle assembly. This setup is shown in Figure 3. This geometry was patterned after the Dresden BWR. The dimensions of 3.7 x 3.7 x 26 cubic inches correspond to the actual 5 pin x 5 pin Dresden fuel bundle. In Figures 3 and 4, the detailed geometry of the spacers between the fuel rods is well resolved by PowerFLOW.

The choice of inlet/outlet boundary conditions for this simulation is the same as in the previous section. Specifically, the coolant flow rate at the inlet (left in Figs. 5 and 6) is set at 4.5ft/sec, and the temperature at 504.8°F. At the outlet, the pressure was set at 990psi. These values are typical for the normal operation regime of the BWR Dresden reactor. The overall resolution of

Figure 3. BWR 5 x 5 Fuel Pin Bundle Geometry.

Figure 4. Close-up view of the fuel pin bundle showing the spacer geometry

Figure 5. Temperature distribution in the longitudinal cross-section of the fuel assembly geometry

Figure 6. Streamlines shade-coded by velocity magnitude in the longitudinal cross-section of the fuel assembly geometry

Figure 7. Close-up view of the exit section of the domain shown in Fig. 6.

Fig. 8a.

Fig. 8b.

Figure 8. Temperature distribution in the fuel assembly transversal cross-section at $h=.25H$ (Fig. 8a) and $h=.75H$ (Fig. 8b).

Fig.9a.

Fig. 9b.

Figure 9. Streamlines shade-coded by velocity magnitude in the fuel assembly transversal cross-section at $h=.25H$ (Fig. 9a) and $h=.75H$ (Fig. 9b).

the simulation is 97x97x684 (number of lattice cells). Figures 5-7 show, respectively, the resulting flow temperature and velocity distributions in a longitudinal fuel assembly cross-section, while Figures 8 and 9 show these quantities at two different transversal cross-section locations. The cross flow patterns are clearly visible. In addition, one can also see the effect of coolant heating by the fuel rods. The temperature field calculated here captures the complex longitudinal and transversal distributions typical for a BWR fuel assembly including the effect of the spacer grids. The demonstrated capability of the new LB approach to simulate such a thermal flow situation is quite important for BWR phenomena.

Simulation of thermo-hydrodynamic phenomena involving vaporization and bubble formation

To demonstrate our novel approach for simulation of non-ideal gas flows, we computed water-vapor phase transition in a vertical heated channel. Subcooled single phase liquid entering at the bottom of the pipe is heated by the heat flux received from the walls as it moves upwards, and begins to vaporize. The vapor leaves the vertical heated channel at the upper end. Although the algorithm developed in Phase I is applicable to full 3-D flow situations, in the initial calculations we have studied a 2-D geometry which at sufficiently high resolution and at sufficiently high Reynolds numbers, allows us to obtain prototypical results with a high computational efficiency. Below we present computational results obtained using 265x2048 grid points. The case set up is defined as follows:

- 1) At the inlet, a high density and low temperature fluid (pure water phase) is injected at a fixed low speed. The velocity profile at the inlet cross section has a parabolic shape according to a fully developed channel flow.

- 2) The side solid walls of the channel are no-slip, water wetting, and fixed heat flux. The heat flux value is chosen in such a way that boiling occurs in the upper part of the channel, as expected in a real BWR fuel bundle.
- 3) The outlet is governed by a free exit condition. That is, either water or vapor from the upper stream can exit the channel while the pressure at the outlet is self-consistently determined via the mass flux constraint based on the inlet values.
- 4) The equation of state used in the simulation is Van der Waals and the constant heat capacity is used for simplicity reasons.
- 5) The initial conditions are chosen to represent a coolant channel filled with single phase subcooled water at the beginning of a simulation.

The spontaneous formation of two-phase flow patterns is illustrated in Figures 10a-d which show the evolution of the fluid density distribution at four consecutive time instants. The plotted values are normalized by the density value at the critical point ($\rho(x,t)/\rho_c$). One can clearly see the coolant separated into high density water (dark shade) phase and low density vapor (light shade) phase having sharp interfaces. The resulting density ratio between the water and the vapor phase varies from 4 to 10. The initial condition used in this simulation corresponds to the entire channel being occupied by the water phase at time zero. Due to the heating of the coolant by the solid walls, the vapor phase emerges first at the outlet of the channel as shown in Fig. 10a. This figure presents a time snapshot of density distribution illustrating the emergence of vapor at

Fig 10a.

Fig 10b.

Fig 10c.

Fig 10d.

Figure 10. Time evolution of the liquid coolant boiling process in a vertical channel with heated walls calculated by the new LB code. Density distributions at four consecutive time are shown.

Fig 11a.

Fig 11b.

Fig 11c.

Fig 11d.

Figure 11. Time evolution of the liquid coolant boiling process in a vertical channel with heated walls calculated by the new LB code. Temperature distributions at four consecutive time are shown.

the outlet corner of the channel as well as appearance of two small bubbles on the left wall. The location of bubble formation is influenced by the random seeding of vapor nuclei near the wall. In time, these bubbles grow, coalesce into larger bubbles, and eventually form continuous vapor regions as shown in Figures 10b-d. Notice that new bubbles appear on both walls at later times.

We have investigated the flow sensitivity to the choice of inlet flow rate, the amount of heat flux from the side walls, wetting properties, and the seeding rate of vapor nuclei, as well as the choice of fluid type such as the equation of state. We have found that if the parameter values are not properly selected, the channel could end up all vaporized or fill with water phase at all times.

The correct implementation of the pressure expansion term in Eq. 6 was found to play an important role in modeling of the latent heat effects. Heat capacity effects are also playing an important role. We have also found that achieving sufficient size and resolution in these multiphase simulations is critical for proper modeling of the effects of statistical fluctuations. Indeed, only at high enough resolution sufficiently small vapor bubbles can be numerically produced in the channel. In addition, it is important to attain sufficient flow rate and Reynolds numbers so that the bubbles can be washed off the wall once they are formed. In this way artificial heat supply to the vapor regions can be avoided and bubble growth and coalescence are simulated more realistically. Figures 11a-d are the plots of temperature distributions at different times corresponding, respectively, to the density distributions shown in Figures 10a-d. Similar to the density, here we have normalized the temperature via its critical point value, $T(x,t)/T_c$. One interesting phenomenon that we have observed is that there is a drop of temperature value in vapor domains at the immediate vicinity of the water interfaces. This temperature decrease obtained in the vapor phase is likely due to the intrinsic latent heat mechanism imbedded in the lattice Boltzmann approach as well as in the energy equation (as mentioned elsewhere in this Report, the lattice Boltzmann algorithm has a built-in surface tension). These physical mechanisms are important for simulating the water/vapor phase transition in order to maintain the proper temperature drop during vaporization.

Summary of Phase I achievements

During Phase I we have completed an analytical formulation of the novel algorithm for simulations of multiphase fluid flows coupled with dynamic heat transfer. The basic algorithm is

a hybrid approach that couples the multiphase lattice Boltzmann algorithm (1, 4) with a finite difference solver of a scalar equation for temperature evolution (6). The tests have proven the usefulness of this approach. Our algorithm is simple, stable, and capable of capturing all the essential physics of multiphase flows involving heat transfer, boiling initiation, and liquid/vapor flow regime formation, making it a perfect candidate for realistic BWR applications.

The Phase I work has demonstrated the viability of our novel approach for multiphase flow simulation. This novel approach has unique potential to become an essential modeling tool for BWR analyses. The remaining issues worth addressing in future research and development involve implementation of realistic equations of state as well as other thermodynamic properties, increasing the stability range and density ratio, implementation algorithm of our algorithm in arbitrary geometries, software parallelization issues, development of a user-friendly general user interface, and testing of realistic BWR flow cases.

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