APPLICATION OF THE LATTICE BOLTZMANN METHOD FOR ONE- AND TWO-PHASE FLOW PROBLEMS
PhD Theses

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Background of research

The accident of the second unit of the Three Mile Island nuclear power plant (TMI-2) in 1979 called attention to the importance of the analysis of two phase flows. Two-phase, one-dimensional system codes used in safety analysis began to be developed in that period. In 2000, the need emerged at AEKI to develop their own real-time, full scope simulator code which can be implemented to the Paks full scope simulator. During the development of this code (RETINA) [10, 11, 12, 13], in which I was also involved, we encountered several problems. The tests revealed that the accuracy of correlations used in the two-phase flow codes is questionable in many cases. Much of the problems arise at the modeling of the mass, momentum, and energy transfer through the interface [10]. After the development of RETINA code, my interest turned to the understanding of the detailed numerical description of the one and two phase thermohydraulical processes. Due to the intensive development of computers, robust program systems - requiring large demand of resources - play more increasing role in computational fluid dynamics recently. These codes are collectively called CFD (Computational Fluid Dynamics) codes.

Research methods

In the last decade a new numerical method emerged in the field of fluid flow modeling. It is commonly called the Lattice Boltzmann Method (LBM). The method itself can be derived from the Boltzmann equation and it is suitable to solve numerically the Navier-Stokes equations. One of its advantages is that its extension for two-phase flow simulation is straightforward and by means of this method the transport through the liquid-gas interface can be investigated in detail. Further advantages are that it can be implemented rapidly and it can be used for investigation of flows in complex geometries [Treeck et al., 2007]. I chose the application of the lattice Boltzmann method as a central issue of my thesis because of the the favorable properties outlined above. During my research I tried to answer questions that are partly related to the characteristics of the method and partly to the basic research in the nuclear industry.

Objectives

Turbulent fluid flow simulation can be carried out at three main levels. These levels vary significantly in the mesh resolutions and in the accuracy of the calculations. The common property of each level is that they solve the Navier-Stokes equations with an appropriate numerical method.

The first such level is called direct numerical simulation. It solves the Navier-Stokes equations directly, without any simplification by resolving the flow down to the size of the smallest eddies. This method gives the most exact result but at the same time, this method requires the largest computational resources. Therefore, only low Reynolds number turbulent flows can be investigated by this method.

The second level of modeling is called large eddy simulation. It still resolves the flow well and under the resolved scales - where the processes are universal - it uses in general a simple turbulence model.

The third widely used level (which has practical relevancy) for turbulent modeling is the so called Reynolds Averaged Navier-Stokes Simulation (RANS). One of its advantages is that by the help of this level very complex geometries can be modeled by the resources available nowadays. However it has the drawback that in order to guarantee the accuracy attention has to be paid to the choice of the turbulent model and its parameters.

Using the lattice Boltzmann method successful simulations have already been carried out at all the three aforementioned levels. The main objective of my work was to develop a two and three-dimensional lattice Boltzmann code that is appropriate for the simulation at direct numerical and at large eddy levels. Two-phase flow modeling in nuclear industry has high relevance. Accordingly, a further code development was aimed at, which is able to the direct numerical simulation of two-phase flows.

One has to verify the operation of the developed codes. Accordingly, the fluid was accelerated between two infinite parallel plates (periodically coupled box) in which the vector of the body force was parallel with the plates. This test has been widely used because it has simple solution in laminar case, and therefore the functionality of the code is easy to prove.

Although numerous successful direct numerical simulations were carried out (the applicability of the method at this level was proved), I aimed to perform turbulent flow simulations between parallel plates for the demonstration of the functionality of the code. A further reason for performing the direct numerical simulation of flow between parallel plates is that this is one of the most well-documented test cases in the literature.

The thermohydraulical processes in a VVER-440 type fuel rod bundle have been an intensively researched field of nuclear industry. The geometry of the real system is very complex, and the nominal Reynolds number of the flow is above 200000, so the fine scale simulation of the rod bundle is not possible. However, it is possible to carry out the investigation of an infinite rod bundle section similar to the VVER-440 geometry at much lower Reynolds number than at nominal conditions.

I investigated the main properties of the flow in the simplified VVER-440 geometry above. The code was validated for laminar case first.

Second, direct numerical simulation of the rod bundle section was carried out at low, but already turbulent Reynolds number region. The main question was whether or not the simulation gave back the basic properties of the flow (secondary flow, flow pulsation phenomenon).

Afterwards, large eddy simulations were performed at larger Reynolds numbers (12000 and 24000). Measurement data were available at these Reynolds numbers, making it possible to check the results. In turbulent case not only the mean quantities of the velocities but also the mean value of the fluctuating velocity components are also important. They are the components of the Reynolds stress tensor, whose investigation was also carried out.

In two-phase flow numerical investigations one of the most important test is the validation of the coexisting curve. Starting from metastable state a small density perturbation is needed for this investigation, which causes phase separation. At a given temperature in equilibrium, maximum and minimum density points appear, which determine two points in the coexistence curve.

The most popular two-phase method in the field of lattice Boltzmann was published by Shan and Chen [Shan and Chen, 1993]. It was observed by Qian and Chen [Qian and Chen, 1997] in one dimension and by Imre and Házi [Imre and Házi, 2002] in two dimensions that the developed coexistence curve depends on the refinement of the domain even in the case of periodic boundary condition. They found that the model of Shan and Chen gives correct coexistence curve only above a given resolution. The need to investigate the problem in three dimensions arose with the developed three-dimensional program system. I investigated whether the finite size effect appears or not and if yes, what minimal resolution should be used to avoid this problem.

In connection with the two-phase lattice Boltzmann methods researchers observed that the developed liquid-gas interface is relatively wide. For instance, the interface of a bubble with a diameter 20 lattices, simulated with the Shan-Chen model cannot produce an interface thicker than three or four lattices because of stability problems. In practice, however, in the case of a macroscopic size bubble the liquid-gas interface falls into the nanometer range - except in the vicinity of the critical point. Consequently, the need to answer the following question arose: does the profile of the developed interface agree with the theoretical one and with the measured data? If the answer is yes, considering the thickness of the interface as a yardstick, what physical size corresponds to one lattice in the real world?

Theses

1. I was the first to carry out direct numerical simulation of an infinite triangular arrayed rod bundle section with the D3Q19 [1, 2] and with the D3Q27 lattice models [2, 3, 4], at 3680 Reynolds

number with the LBM3D1P owned developed, one-phase, three-dimensional, lattice Boltzmann code.

a. Validating the code the results of the lattice Boltzmann method were compared to analytical solutions in laminar case. During the calculations both the results of the D3Q19 and the D3Q27 model was examined [2, 4]. It was found that the relative error of the axial velocity is the highest at the wall and away from the wall the error decreases significantly. The maximal error is below 2%.

b. Direct numerical simulation was performed with the validated code at Reynolds number 3680. The time-averaged lateral velocities showed secondary flow [2, 3, 4].

2. It was my experiments that large eddy simulation of an infinite triangular arrayed rod bundle section was first carried out with the D3Q19 [1, 2] and with the D3Q27 lattice models [1, 2, 3, 4, 5, 6], at 12000 and at 24000 Reynolds numbers with the LBM3D1P code.

a. Using the D3Q27 lattice model the mean lateral velocities show secondary flow cells in each thirty degree segment of the subchannel correspondingly with the measurements [2, 3, 4, 5, 6].

b. The mean axial velocities carried out by the D3Q19 lattice model simulations, in contrast to the D3Q27 lattice model, showed qualitatively incorrect result [2, 3]. The simulation did not give back the desired 60 degree symmetry of the system. This was observable at both the direct numerical and the large eddy simulations, it can be excluded that the turbulent model played a role in the incorrect mean axial value in the large eddy simulation.

c. The (UV) component of the Reynolds stresses are in good agreement with the measurement published by Trupp and Azad [Trupp and Azad, 1975], except in the vicinity the of wall [5, 6]. It can be stated that the accuracy increases with the grid refinement. The normal stresses (RMS - root mean square) in the bulk are also in good agreement with the measurements. In the vicinity of the wall, however, because of the lack of wall function or refinement of the wall, significant deviation can be seen.

3. Infinite liquid-vapor interface evolving in the x-y plane and perpendicular to the z plane was modeled in equilibrium by the lattice Boltzmann method. For the investigations I used the LBM3D2P, three-dimensional, two-phase program system, which uses the model of Shan and Chen [7, 8].

a. Numerical calculations showed that the interface profile simulated by the lattice Boltzmann method is in good agreement with the theoretical tangent hyperbolic profile and with the measurements.

b. This allowed to determine the size of one lattice cell in lattice Boltzmann simulations using the thickness of the interface . The results made by the lattice Boltzmann code were compared to those coming from the molecular dynamical simulations of argon. It was found that the size of one lattice Boltzmann cell is approximately 36 nm.

c. When the thickness of the interface has to be taken into account, macroscopic size interface can be modeled with the method of Shan and Chen only in the vicinity of critical point.

4. The effect of the three-dimensional refinement of the domain to the coexistence curve was investigated in a periodic box by the lattice Boltzmann method [9] using the LBM3D2P two-phase code. The method proposed by Shan and Chen was applied to the simulations.

a. In three dimensions the results of the simulations justified the finite size effect to the coexistence curve, observed in one and two dimensions already.

b. It was found that the coexistence curve is in good agreement with the corresponding equation of state at resolution 40x40x40.

c. The coexistence curve produced by the three-dimensional simulations converges to that two-dimensional. Consequently, when only the coexistence curve has to be determined it is enough to carry out two-dimensional simulations instead of the three-dimensional simulations needing large computational resources.

References to theses

- [1] P. Kávrán, G. Mayer, G. Házi, Nuclear Energy for New Europe 2003, Portoroz, Slovenia, September, 2003
- [2] G. Mayer, G. Házi, Direct numerical simulation of longitudinal flow along triangular array of rods using the lattice Boltzmann method, The 14th International Conference on Discrete Simulation of Fluid Dynamics in Complex Systems, Kyoto, Japan, August 22-26, 2005
- [3] G. Házi, G. Mayer, Flow in rod bundles, Nuclear Energy for New Europe 2005, Bled, Slovenia, September 5-8.
- [4] G. Mayer, G. Házi, Direct numerical and large eddy simulation of longitudinal flow along triangular array of rods using the Lattice Boltzmann method, Mathematics and Computers in Simulation, Vol.72, 173-178, 2006
- [5] G. Mayer, J. Páles, G. Házi, Large eddy simulation of subchannels using the lattice Boltzmann method, Annals of Nuclear Energy, 34, 140-149, 2007
- [6] G. Mayer, Large eddy simulation of a fuel rod subchannel, ICONE15, 15th International Conference on Nuclear Engineering, April 22-26, 2007, Nagoya, Japan
- [7] G. Mayer, G. Házi, J. Páles, A. R. Imre, B. Fischer and T. Kraska, On the system size of lattice Boltzmann simulations, International Journal of Modern Physics C., Vol.15, No. 8, 2004
- [8] G. Mayer, G. Házi, A. R. Imre, B. Fischer, J. Páles and T. Kraska, Lattice Boltzmann and molecular dynamics simulation: on the size of mesoscopic systems, 3rd International Workshop "Global Phase Diagrams", Sept. 14-19, Odessa, Ukraine, 2003
- [9] G. Mayer, G. Házi, A. R. Imre, T. Kraska and L. V. Yelash, Lattice Boltzmann simulation of vapour-liquid equilibrium on 3D finite lattice, International Journal of Modern Physics C., Vol. 15, No. 3, 2004

Other references

- [10] G. Házi, G. Mayer, I. Farkas, P. Makovi and A. A. El-Kafas, Simulation of a small loss of coolant accident by using RETINA V1.0D code, Annals of Nuclear Energy, Vol.28, 1583-1594, 2001
- [11] G. Házi, G. Mayer and I. Farkas, RETINA V1.0D Kétfázisú áramlásokat modellezõ programrendszer, Magyar Energetika 1, 2001

- [12] I. Farkas, G. Házi, G. Mayer, A. Keresztúri, Gy. Hegyi and I. Panka, First experience with a six-loop nodalization of a VVER-440 using a new coupled neutronic-thermohydraulics system KIKO3D-RETINA V1.1D, Annals of Nuclear Energy, 29, 2235-2242, 2002

- [13] G. Házi, I. Farkas and G. Mayer, RETINA: A new simulator code for two-phase flow modeling, Int. Conf. on Supercomputing in Nuclear Applications SNA2000, Toranamon-Pastoral, Tokyo, Sept 4-7, 2000

- [14] E. Végh, G. Házi, J. S. Jánosy, G. Mayer, L. Seregi, B. K. Szabó, Graphical Simulator of the ETTR-1 Research Reactor, 15th European Simulation Multiconference, Jun. 6-9, Prague, Czezh Rep., 2001

- [15] G. Házi, I. Farkas, G. Mayer, Kétfázisú áramlások modellezésének fizikai és numerikus kérdései, KFKI AEKI Tanulmány, OMFB Részjelentés, 1999 ALK-00093/98/1, 1999

- [16] G. Házi, I. Farkas, G. Mayer, P. Makovi, RETINA: Two-phase Thermohydraulics for NPP Simulators (1999), AEKI Progress Report, pp. 23

- [17] G. Házi, I. Farkas, G. Mayer, RETINA: Termohidraulikai és szoftver rendszerterv, ALK 00093/98/2, 1999

- [18] G. Házi, G. Mayer, RETINA: Benchmark feladatok elõzetes kidolgozása, OMFB részjelentés, ALK-00093/98/3, 1999

- [19] G. Házi, I. Farkas, G. Mayer, RETINA: A fizikai és numerikus tesztek eredményei, OMFB Zárójelentés 2000, ALK-00093/98

- [20] A. R. Imre, G. Mayer, G. Házi, F. Römer, R. Rozas, T. Kraska, Determination of the spinodals of pure fluids from interfacial properties: molecular dynamics an Lattice Boltzmann Simulations, European Symposium on Applied Thermodynamics, Cannes, May/June 2008

- [21] G. Mayer, Coherent Structures in rod bundle flows: Lattice Boltzmann simulation, The Fourth International Conference for Mesoscopic Methods in Engineering and Science, July 16-20, 2007, Munich, Germany

- [22] A. R. Imre, G. Mayer, G. Házi, R. Rozas, T. Kraska, Estimation of the liquid-vapor spinodal from interfacial properties obtained from molecular dynamics and lattice Boltzmann simulations, The Journal of Chemical Physics, 128, 114708, 2008

- [23] T. Kraska, L. V. Yelash, A. R. Imre, G. Házi, G. Mayer, Fluid-fluid phase transitions in pure binary liquids, DFG-OTKA Workshop on Promoting Hungarian-German Cooperations in Physics, May 2003, Budapest

- [24] A. R. Imre, G. Mayer, G. Házi, R. Rozas, T. Kraska, Estimation of spinodals in pure fluids from interfacial properties obtained from equilibrium molecular dynamics and lattice Boltzmann simulations, DPG-Frühjahrstagung, Berlin, Februar 2008

- [25] A. R. Imre, G. Mayer, G. Házi, R. Rozas, T. Kraska, Abschätzung der Spinodalen von fluiden Reinstoffen aus Grenzflächneigenshaften: Molekulardynamische und Lattice Boltzmann Simulationen, Bunsentagung, Saarbrücken, May 2008

- [26] G. Házi, A. R. Imre, G. Mayer and I. Farkas, Lattice-Boltzmann methods for two-phase flow modeling, Annals of Nuclear Energy, 29, 1421-1453, 2002

- [27] G. Mayer, G. Házi and I. Farkas, Determination of pressure loss coefficient of a VVER-440 steam generator with lattice Boltzmann simulation, Bridging the time-scale gap, Sept 10-13, Konstanz, Germany, 2001
- [28] G. Mayer, Falsúrlódásból származó nyomásesés vizsgálata egy VVER-440 típusú gõzfejlesztõ köpenyterén keresztül, háromdimenziós rács-Boltzmann módszer segítségével, Nukleáris Technikai Szimpózium 2002, Budapest, 2002. október 3-4.

References

[Imre and Házi, 2002] Imre, A. R. and Házi, G. (2002). The effect of finite lattice-size in lattice Boltzmann model. *Int. J. Mod. Phys C*, 13(5):649–657.

[Qian and Chen, 1997] Qian, Y. H. and Chen, S. (1997). Finite size effect in lattice-BGK models. *Int. J. Mod. Phys. C.*, 8(4):763–771.

[Shan and Chen, 1993] Shan, X. and Chen, H. (1993). Lattice Boltzmann model for simulating flows with multiple phases and components. *Phys. Rev. E*, 47(3):1815.

[Treeck et al., 2007] Treeck, C., Hillion, F., Cordier, A., Pfaffinger, M., and Rank, E. (2007). Flow and thermal sensation analisys in an aeroplane passenger cabin using lattice Boltzmann based approach. *International Conference for Mesoscopic Methods in Engineering and Science*.

[Trupp and Azad, 1975] Trupp, A. C. and Azad, R. S. (1975). The structure of turbulent flow in triangular array rod bundles. *Nucl. Eng. Des.*, 32:47.