Hygrothermal simulation and risk evaluation - A literature review and assessment of the applicability of the Lattice Boltzmann Method to derive the influence of convection on moisture behaviour in building components

A Sarkany [1] **and T Bednar** [1]

[1] Institute of Material Technology, Building Physics, and Building Ecology, TU Wien, Vienna, Austria

E-mail: `andreas.sarkany@tuwien.ac.at, thomas.bednar@tuwien.ac.at`

Abstract. Since the Lattice Boltzmann Method (LBM) showed promising ways in describing fluid flow and convective phenomena, this literature review gives an overview of the application of LBM to date in the realm of hygrothermal simulations (HAM). Furthermore, ways to apply LBM to derive the influence of convection on moisture transport in building components are assessed. This is achieved by a literature review which is carried out for specific fields of application of LBM which are intertwined with topics of hygrothermal simulations (Natural convection, Porous media, Flow through channels). The introduction is accompanied by a condensed theoretical overview of the used LBM-scheme in most of the reviewed literature. It could be seen that, in regard to these topics, the majority of simulations is carried out 2-dimensionally using mostly the D2Q9 model with single relaxation times. The reviewed literature shows LBM as a validated tool, solidifying the choice of LBM for our purposes. No coupling of LBM to HAM-simulations to derive the influence of convection on moisture transport could be found. In conclusion, the deduction of parameters like the permeability is identified as a potent subfield for the coupling of LBM and HAM-simulations for further research.

1. Introduction

In the last two decades the Lattice Boltzmann Method proved to be a helpful tool when studying the behaviour of flows in the mesoscopic domain in a variety of fields, covering a wide range from medicine [1], to geology [2], to material technologies [3]. Although first steps have been taken to apply this method in the realm of building physics [4, 5, 6], the most potent subfields of application have yet to be defined. Generally, the problems studied in building physics take place on the macroscopic domain, therefore, the mesoscopic scale on which the Lattice Boltzmann Method operates suggests to use it as a pre-analysis of certain parameters which later can influence the results on the macroscopic field, Figure 1. In building physics, the subfield of hygrothermal simulations relies strongly on material parameters and their exact determination, as results of the executed tasks in Annex 41 showed us [8]. Especially the influence of unwanted, naturally occurring convection, is, due to its probabilistic nature, still not implemented into hygrothermal simulation models in sufficient detail [8]. Although convective moisture transport

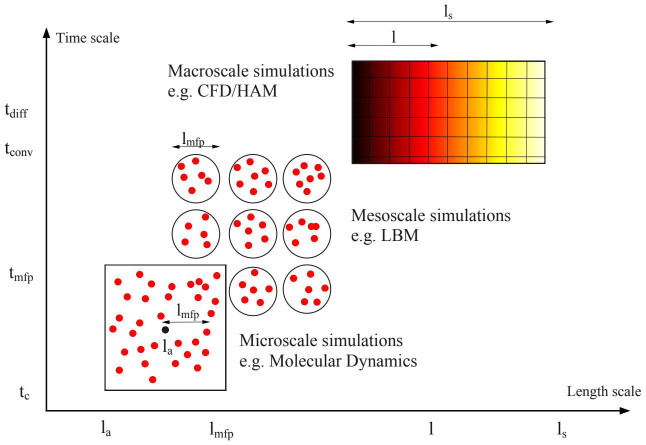

Figure 1. Different time and length scales of problems with the suitable simulation techniques, adapted from Kruger et al. (2017) [7].

has been known as a driving factor in the durability of building components [9, 10] and efforts have been undertaken to take convective moisture flow into consideration [11, 12], current models deal with predefined locations or routes where convective moisture transport occurs. Unwanted, naturally occurring convection, e.g. in gaps and between joints, but also due to craftship, could be defined as one of the known unknowns in the sense of risk characterization by Annex 55 [13] where McManus (2005) is quoted. Their description and modelling could help hygrothermal simulation results to reflect real world behaviour more realistically because "the effects of potential defects are included" [14].
For this review and assessment of the possible application of the Lattice Boltzmann Method to deduce the influence of convection on moisture behaviour in building components, we will look into its potential to better characterize these unwanted, naturally occurring convective phenomena, focusing on air flow through joints and gaps. The listing of our findings will be followed by a summarizing discussion and the derivation of possible fields to apply the method to and the potential problems that could arise by execution.

2. Literature review

To determine possible applications to couple analysis between the mesoscopic and macroscopic scale we review past work where LBM was used in sub-topics which are relevant to the problem. The studied works for this review therefore needed to include one or more of the following topics: *natural convection, porous media, flow through channels and tunnels.* The review was carried out using mostly the following research platforms: *Elsevier, Science Direct, Research Gate, Google Scholar.*

2.1. Introduction - Theoretical overview and terminologies

To easier follow along the results and terminologies of the reviewed papers, a short overview of the reoccurring general theory of the applied LBM and nomenclatures in these works will be given, strongly following the outline given by Mohamad (2019) [15]. The Boltzmann equation without an external force can be written as Equation 1

$$\frac{\partial f}{\partial t} + c \cdot \nabla f = \Omega \tag{1}$$

where f is a distribution function dependant on location x, speed c and time t. Ω is the collision term describing "rate of change between the final status and the initial status of the distribution function" [15]. Due to the complexity of Ω the BGK (Bhatnagar, Gross, and Krook 1954) approximation is used for the right hand side, so it can be rewritten into

$$\frac{\partial f}{\partial t} + c \cdot \nabla f = \frac{1}{\tau} \cdot (f^{eq} - f). \tag{2}$$

The discretization of Equation 2 for specific directions yields in Equation 3 and is commonly referred to as the lattice Boltzmann method.

$$\frac{\partial f_i}{\partial t} + c_i \cdot \nabla f_i = \frac{1}{\tau} \cdot (f_i^{eq} - f_i) \tag{3}$$

Finally, for the numerical implementation, Equation 3 can be discretized into Equation 4, sometimes also referred to as a finite difference discretization of the discrete Boltzmann equation rephrasing Sousa and Nabovati (2008) [3] citing Geller et al. (2006).

$$f_i(\vec{x} + \vec{c}_i \Delta t, t + \Delta t) - f_i(\vec{x}, t) = \frac{\Delta t}{\tau} \cdot [f_i^{eq}(\vec{x}, t) - f_i(\vec{x}, t)] \tag{4}$$

For the right hand side of Equation 1 the terms single- and multi-relaxation time (SRT and MRT) are from importance. In Equation 4 a single relaxation time model is used. While the SRT-model is easier to implement MRT offers greater stability but at a higher computational cost [15, 16]. The lattice arrangements and thus the dimension and resulting streamlines are described with the common terminology DnQm, where n stands for the number of dimensions of the problem and m expresses the number of linkages of a point on the lattice [15].

2.2. Natural convection

Natural convection takes place due to thermally induced density differences, therefore it can lead to unwanted convective mass transport even though the air tightness of the building envelope is ensured. When deducting studies in regard to natural convection with LBM 3 main topics of interest could be identified: Study of natural convection in square cavities, study of natural convection in regard to porous media, studies of the use and innovation of coupled LBM - finite difference/volume methods for natural convection simulation.

2.2.1. Natural convection - Square cavities

The study of natural convection in square cavities examines simulation results for the given domain in regard to dimensionless numbers, like the Rayleigh (Ra), Prandtl (Pr), Nusselt (Nu) or Reynolds (Re) number. The usual model and different variations of problems are depicted in Figure 2. The results are compared and validated to benchmark cases and data from the literature. For the investigation of natural convection in square cavities, only dependant on uniform boundary conditions, the multiple-relaxation time lattice boltzmann method (MRT-model) proved to be in well agreement with referenced solutions [17, 18].

Heat emitting obstacles where part of investigations in the following works and dealt with different locations and geometries for the obstacles in the simulation domain. Bararnia, Soleimani, and Ganji (2011) [19] studied the influence of the position of a heated elliptic inner cylinder in a square outer cylinder numerically. The investigation showed that the results strongly depend on the location of the heated inner cylinder and the Rayleigh number ranging from 10^3 to 10^6. While Goodarzi et al. (2018) [20] developed a nano scale method for LBM, Imani (2020) [21] and L. Wang et al. (2019) [22] looked into the application of LBM for conjugate natural convection with square and cylindrical obstacles.

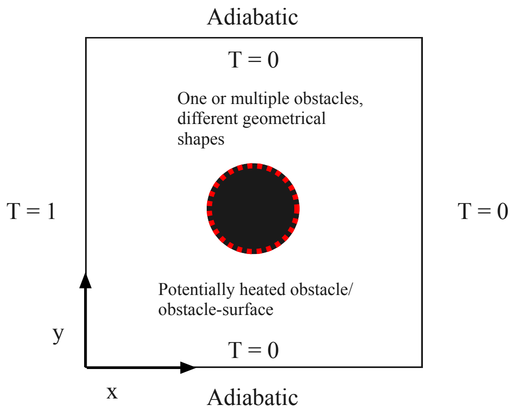

Figure 2. Usual model configuration for examining the behaviour of natural convection. The complexity rises from no obstacle to a heated obstacle in the simulation domain while the configuration of heat and sink sources and geometrical shapes of the obstacle may also vary.

2.2.2. Natural convection - Porous media

Studying porous media either the flow through or around the media and the influence of the porous matrix on its behaviour is analysed. By applying a single relaxation time model He et al. (2020) [23] analysed fluid flow, heat and mass transfer in heterogeneously porous media with the effect of temperature-dependent viscosity. The results showed that the buoyancy ratio influences the effect on porosity on heat and mass transfer in the cavity and the convection mode in the porous media [23]. Computer tomography is often used to capture the porous domain [24, 25, 16]. Also by Yun et al. [24] "X-CT has been used to obtain a 2D optical image of various slice with different location". Out of this data the model for the porous medium could be created. The impact of higher Rayleigh and Prandtl numbers on flow and heat transfer could be observed. Zhao et al. used a double-populations model to "simulate the natural convection in a square cavity filled with square and circular metal blocks" [26]. It was discovered that the metal porous medium enhanced the natural convection in a square cavity. Moreover it was stated "porous medium enhances the natural convection in a square cavity. The heat transfer is enhanced with the increase of the pore density, however it is weakened with the increase of the porosity." [26]. Dealing with the effects of porous layers and their influence on heat transfer and flow in [27, 28] the following conclusions where deducted. The covering of a cylinder wall by a porous layer "can change the flow pattern and enhance the heat transfer" [27], but this effect lessens at lower Rayleight numbers($\mathrm{Ra} = 10^3, 10^4$). In both works it is stated that an increase in the Darcy number leads to an increase in the average Nusselt number [27, 28]. Hu et al.(2016) [27] also could obtain "a critical value of the thermal diffusivity for a porous layer of given thickness, above/below which heat transfer augmentation/reduction will be obtained, and the critical value decreases with increasing Rayleigh number or decreasing Darcy number." [27].

2.2.3. Natural convection - Coupled analysis

For coupled or hybrid analysis the finite volume and finite difference method were proposed to simulate natural convection [29, 30, 31]. In Nee (2020) [30] fluid flow was solved with LBM "under Bhatnagar-Gross-Krook approximation with D3Q19 scheme" while "unsteady three-dimensional energy equation was solved by means of the finite difference technique". "When $\mathrm{Ra} = 10^3$, $\mathrm{Ra} = 10^4$ and $\mathrm{Ra} = 10^5$, computational performance of hybrid lattice Boltzmann method was correspondingly 38, 29 and 19 times higher than conventional CFD approach." [30]. Polasanapalli and Anupindi (2019) [31] present a CFDLBM framework to simulate thermal flows. The higher-order compact-schemes employed in this work could lead to the lower mesh resolutions needed for the simulations. Li, Yang, and Zhang (2014) [29] propose a coupled LBM and FVM method for the fluid heat transfer problem. The results of variations of the coupled method are compared to the results of the isolated methods and in good agreement with each other [29].

2.3. Porous media

Most materials used in construction are of porous nature and especially in HAM a lot of material properties and their behaviour (e.g. liquid water transport) are influenced by this [32]. For porous media the majority of the studies can be structured into the following reoccurring topics of interest: heat and moisture convection, deduction of parameters for transport processes, drying, coupling of LBM with pore networks.

2.3.1. Porous media - Heat and moisture convection

Intertwining goal when looking into heat and moisture convection in porous media is the derivation of a deeper quantifiable understanding of these processes as an underlying foundation to build upon for further examinations. Sheng Chen, W. Li, and Mohammed (2021) [33] develop a new approach to simulate natural convection of large Pr-number fluids in porous media. They present four novel findings, one of them being "there are three characteristic zones and two critical Prandtl numbers for natural convection of large Prandtl number fluids in porous media. The dominant heat transfer mechanisms in these zones are completely different, so the variation trends of the correlation between Nu and Pr in these zones are different" [33]. The main effects of porous material in a square cavity are stated as follows in [34]: "By increasing porosity, the heat penetration in different parts of the cavity is reduced. More uniform heat distribution and elimination of hot zones in the cavity is observed by increasing porosity and reducing Richardson number." LBM was used and adapted to investigate double-diffusive convection in fluid-saturated porous media in [35] and for arbitrary combinations of solid, fluid, and porous media in [36]. Both models are in good agreement with their validation cases and are therefore proposed for their respective problems [35, 36]. The applied usage of LBM for engineering question was shown in [37],where LBM was used to simulate the effective heat transfer through vacuum insulation.

2.3.2. Porous media - Deduction of parameters for transport processes

The reverse engineering of parameters for transport processes showed promising results over the years, predicting permeability [25, 38, 3, 16]. The method applied, while differing in the details of the specific simulation parameters used for LBM, relies on modelling the pore structure either based on real depiction [25, 16] (eg.micro-CT, observation) or random generation [38, 3, 16], simulating the particle flow through the medium and calculating the wanted parameters based on the behaviour/results obtained.

2.3.3. Porous media - Drying

The results in regard of drying in porous media using LBM are from interest because often in these models the behaviour of particles in contact with the surface layer and its modelling is discussed. Numerical simulations of drying of deformable anisotropic porous medium were conducted in [39]. Due to short falls of pore network models LBM was used in [40, 41] to simulate drying of capillary porous media. Panda et al. (2020) [40] investigate the complex multiphase-multicomponent process in capillary porus media and LBM is showcased as a proof of concept for drying problems. The advantages of LBM for the investigation of drying of capillary porous media suggest "to incorporate LBM into PNM to make it more efficient i.e. by intelligently switching to LBM during capillary unstable regimes." [41].

2.3.4. Porous media - Coupling of LBM with pore networks

The accuracy but computational expense of LBM compared to the efficiency yet lower accuracy of PNMs [26] has drawn attention to the coupling of the two methods. "To describe the throat structure more accurately, the throat bonds with real cross sections are retained in the improved pore network model." [42]. Then LBM is used to calculate arbitrary throat bonds, while efficiency is improved by the use of artificial neural network models [42]. Furthermore, 3 different improved pore network models are presented in [43], where a MRT single phase LBM again "is used to simulate fluid flow in the throat bonds and calculate their conductances".

2.4. Flow through channels

Since the flow through gaps and joints between building parts could be a potential source for unwanted moisture convection, we looked into different usages of LBM to analyse flow through gaps and cavities [44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54]. Investigations of different Re numbers in constricted and straight channels indicate that the "average flow resistance increases and the heat transfer rate decreases in a constricted channel in comparison to a straight channel" [45]. Javadzadegan, Motaharpour, et al. (2019) [48] outline some key findings when investigating the radiative-convection heat transfer in a channel. These findings can be used to check the behaviour of self developed models for plausible behaviour. If looking at differentially heated walls in a micro channel Javadzadegan, Motaharpour, et al. (2019) [48] found "that the Knudsen number has important role in heat transfer". For particle transport in a turbulent channel flow "The simulations show that the Stokes number, St, mass loading of particles, i.e. ratio of mass of dispersed to carried phase, mp=mf, and particle diameter, dp, are important parameters that determine the distribution of the particles and the impact of the particles on the fluid velocity flow field." [50]. Thermal diffusivity could be deduced as an important factor for the conjugate heat transfer rate through a wall obstacle in a channel [51]. Simulations through different geometrical shapes of tubes have been conducted by Najafi, Naghavi, and Toghraie (2019) [52] leading to the observation that the shape of the hydrodynamic channel affects the turbine efficiency. For staggered tube banks the results in [53] show that D3Q27 and D3Q19 lattice model do not differ significantly for these problems. Computational performance of different LBM implementations was investigated in [44] while Jadidi et al. (2022) [47] can be consulted for optimal relaxation times for different Re numbers.

3. Findings and Discussion

For the 3 topics this literature review is focusing on, it can be summarized that when LBM was used in the conducted studies good agreement with benchmark cases and/or data from the literature could be achieved. Therefore, it can be said that the Lattice Boltzmann Method is a sufficient tool for analysing these topics. Figure 3 shows the reviewed papers in regard to our researched topics ordered in the period of their release year. It can be seen that, for all applications looked at in this review, the majority of the reviewed papers was released between 2016 and 2021. In Table 1, a summary of different LBM schemes used in the fields of application, when it was available, is given as a qualitative overview. It can be seen that the majority of simulations in these topics were carried out 2-dimensionally using mostly the D2Q9 model with single relaxation times. It can be assumed that this is due to the complexity of implementation of a 3D or multi-relaxation time model, but also because for most of the questions in these works the chosen dimension and scheme were sufficient for solving those problems. The well documented and validated cases when looking at natural convection solidify the hypothesis to

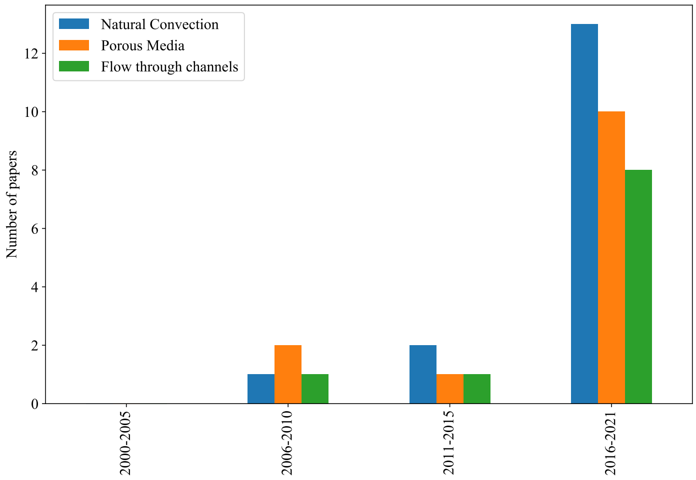

Figure 3. Papers of this review in regard to the review topics ordered in the period of their release year. It can be seen that the majority of the publications found have been from the last 5 years.

Table 1. Different LBM schemes used in regard of the different fields of application.

	D2Q4	D2Q5	D2Q6	D2Q9	D3Q15	D3Q19	D3Q27	SRT	MRT	Multiple population model
Natural Convection	-	-	-	11	-	-	1	10	2	7
Porous Media	-	-	-	5	1	-	-	4	1	1
Channels and Tubes	1	1	1	7	-	2	1	7	1	5

choose LBM as a tool to look into these problems for our research question. From Tiftikci and Kocar (2016) [53] we can assume that for 3D simulations the D3Q19 model, and based on Table 1 for 2D simulations D2Q9 can be seen as educated guesses and preferable starting points. While coupling with PNMs [55, 42, 43] and FVMs/FDMs [29, 30, 31] could be found, the coupling of LBM to macro-scale simulations (eg. HAM-simulations), which are generally used in building physics, hasn't been found. When investigating LBM for porous media simulation, it was seen that a possibility to form such a coupling would be the deduction of parameters on the meso-scale which later can be applied to the simulations on the macro-scale, where Sousa and Nabovati (2008) [3] and Yin et al. (2019) [56] show very promising applications which could be investigated in future research.

4. Conclusions and Further Research

A literature review on the possible application of the Lattice Boltzmann Method to derive the influence of convection on moisture behaviour in building components was conducted. As a starting point, the review focuses on the topics natural convection, porous media and flow through channels since they seemed to be intertwined in the realm of particle simulations with the research question. The review showed that LBM is a validated tool analysing these topics, while the most potent subfield for coupling meso-scale with macro-scale simulations seems to be the deduction of parameters like the permeability via LBM. The widening of the reviewed topics in regard to the research developments is a future possibility. As a next step, the subset of parameters on the macro-scale for coupling will be evaluated. A possible new numerical method where this coupling of LBM and HAM simulation could be most beneficial will be part of our future work.

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