HEAT AND MASS TRANSFER IN TURBULENT MULTIPHASE CHANNEL FLOW

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Chapter 1

Introduction

1.1 Droplets in turbulent flow

Turbulent multiphase flows with a large number of dispersed droplets in a gas are present in many processes both in nature and in industry. The possible enhancement of heat transfer by the presence of particles is an important aspect in the design of more efficient devices. On larger scales the investigating of droplet dynamics in turbulent atmospheric clouds can help to describe and understand their influence on our climate.

Turbulent flow itself is considered a major problem of classical physics. It can be modeled in various ways and moreover, different numerical and experimental methods were developed during the last century in order to increase our understanding of turbulence. The presence of a large number of particles and droplets in a turbulent flow makes the problem even more challenging from both modeling and computational points of view. Several studies were dedicated to the study of fundamental issues of turbulent droplet dynamics by means of the Lagrangian approach (Shraiman and Siggia 2000, Procaccia 2001). In particular, on the smallest turbulent scales droplets which are heavier than the fluid are propelled away from vortices and gather in regions of strain (Cencini et al. 2006). Moreover, if their volume and mass fraction are sufficiently large, they influence the turbulent flow itself. Particles with different Stokes number, which characterizes how fast the particle adapts to the flow, were investigated in Calzavarini et al. (2008). In Figure 1.1, left we observe that heavy particles are subject to preferential clustering.

The current PhD study is part of a research project called DROP, funded by FOM, the aim of which is a better quantitative and fundamental understanding of the dynamics of droplets in turbulent flows. The project is carried out by research groups in the Netherlands from Delft, Eindhoven and Twente, and includes four experimental and four numerical studies. In particular, the study presented in this PhD thesis concentrates on the mass and heat transfer in droplet-laden turbulent channel flow in which droplets undergo phase transition. The study conducted by Kuerten et al. (2011) showed an enhancement of the heat transfer in turbulent channel flow by more than a factor of two by introducing heavy inertial particles. We take the next step in the physical modeling by introducing phase change between dispersed droplets and carrier gas and investigate its effect on the global heat transfer properties of channel flow and on the droplet behavior. The modeling challenge is to take into account not only the exchange of momentum between the two phases but also of mass and energy, taking the dispersed nature of the liquid droplet phase in the continuous gas flow into account using an

Fig. 1.1: Snapshot of the distribution of heavy particles in a turbulent flow field (right) compared to the case of tracers (left). From Calzavarini et al. (2008) .

Euler-Lagrange formulation (Mashayek 1998, Miller and Bellan 1998).

Before presenting the contents of the thesis, we will briefly discuss the choices which we made in physical modeling and numerical treatment of the problem. Next, the key points of each chapter will be presented along with the general outline of this thesis.

1.2 Models and methods in the context of modern computational capabilities

A turbulent flow can be modeled in various ways. In this thesis we make use of direct numerical simulation in which all scales of the flow, except the detailed flow around each droplet, are resolved. Droplets are solved using the point-particle approach which is common practice when the size of the droplets is smaller than the Kolmogorov scale (Marchioli et al. 2006). This permits to maintain the computational costs within acceptable levels compared to the turbulent flow case but without droplets.

We adopt the Euler-Lagrangian formulation which imposes conservation laws for mass, momentum, energy and species of the carrier phase, while using empirical correlations for the interaction between the two phases. Two-way coupling terms are derived reflecting the interaction of droplets with the carrier gas conserving mass, momentum and energy. The model equations used for the two phases resemble the approach used by Miller and Bellan (1998), Masi et al. (2010).

One of the issues while modeling the carrier gas is whether to use a compressible or an incompressible formulation. The Mach number, which is a non-dimensional parameter characterizing the compressibility of the flow, is very low for the conditions which we simulate. It is approximately equal to 0.005. It is common practice to treat the flow as incompressible for Mach numbers smaller than 0.3 (Anderson 2007). In the present study the carrier gas consists of water vapor and dry air. If the carrier gas is assumed to be strictly incompressible, then all

instantaneous changes in the mass density of vapor and air should cancel each other precisely throughout the domain. A full simulation model was developed for such an incompressible carrier phase by Russo et al. (2014a). Here, we confront the incompressible model with a fully compressible description, which allows to quantify the consequences of non-constant mass density of the carrier phase and indicates in which respects and under what conditions the full compressible formulation becomes essential. While the kinematics of the flow are not very sensitive to the Mach number in the low-Mach regime, more subtle influences, deriving from thermodynamics associated with the phase changes within the flow, display a stronger sensitivity to compressibility.

Another challenge which we face in this study is the choice of a suitable time integration method. We perform the first part of the work using a density-based fully explicit time integration method. In order to avoid excessive computational requirements caused by the stability conditions of this time integration method, this method is applied to low values of the Mach number that are, however, much higher than the actual value of 0.005. In order to enable efficient simulation at the real Mach number we develop a different time integration method which belongs to the class of pressure-based methods for compressible flows. We extend earlier work by Bell et al. (2004) to two-phase flows with phase transitions and validate it using the results of the fully explicit solver.

The study of Russo et al. (2014a) and the first chapters of this thesis consider flows without gravity. If gravity in the wall-normal direction is taken into account, droplets migrate continuously towards the bottom wall and will typically create a film of water there. This motivates us to investigate the extended setting in which initially a thin film of water covers the bottom wall while a large number of droplets is dispersed in the domain. In this work the film is considered to have a constant height and its surface does not move. Moreover, we keep the total mass of water in the system constant by draining water from the bottom wall and inserting, on average, the same amount in the form of new droplets released at the top wall. We investigate in detail the behavior of the droplets along with the heat transfer properties of the channel in the presence of gravity.

1.3 Structure of the thesis

This thesis comprises three main developments in the field of turbulent multiphase flows with phase transitions. These will be discussed briefly next.

1.3.1 Comparison of compressible and incompressible formulations

The second chapter of the thesis is dedicated to the description of the problem and the modeling equations for the two phases using either a compressible or an incompressible formulation for the carrier phase. We investigate the sensitivity of the system to a low level of compressibility by confronting the results from these two formulations. We choose ‘mild’ initial conditions of room temperature, atmospheric pressure and 100% relative humidity in order to guarantee ‘modest’ coupling between the phases expressed by the mass transfer. Consequently, only small differences between the results of the two formulations should be

expected, serving as a point of reference. We concentrate on heat and mass transfer quantities of the channel. The results give evidence of the need for the compressible formulation even for the lowest value of the Mach number of 0.05 investigated. Changes in, e.g., the Nusselt number of up to 15% were observed when the mean system temperature is elevated to about 50 degrees C, while overall the agreement between the two formulations is quite close.

In the third chapter we present the results of a study into compressibility effect due to phase transitions and choose significantly lower values of the initial relative humidity. This has the effect of emphasizing evaporation during initial stages which has a marked influence on droplet sizes and associated heat transfer. We concentrate on the Nusselt number (Kuerten et al. 2011) and analyze all contributions to it. The main finding of this study is a 1.5 larger difference in the Nusselt number between the two formulations in case of initial relative humidity of 50% than in the results for the mild case of a saturated initial state.

1.3.2 Low Mach number time integration algorithm

The fourth chapter of the thesis is dedicated to the new time integration algorithm for low Mach droplet-laden turbulent channel flow with phase transitions. There are two main numerical techniques for the treatment of compressible low Mach number flows: density-based methods and pressure-based methods. Two types of time-marching procedures are applied in density-based methods: explicit and implicit algorithms. The severe restriction on the time step for low values of the Mach number in explicit solvers is dictated by a stability restriction, called Courant-Friedrichs-Lewy (CFL) condition (Morton and Mayers 2005). We faced this problem in the study described in chapters two and three where the fully explicit time integration method applied in the compressible formulation required long computational times. In implicit density-based methods the system of governing equations for compressible turbulent flow is ill-conditioned, making iterative solution methods excessively time consuming (Roller and Munz 2000).

To alleviate these problems for unsteady low-Mach flows we focus on a pressure based method which is very similar to pressure correction methods used for incompressible flow. We apply this method to a system of equations obtained by asymptotic analysis at low Mach numbers. The main virtue of this approach is the absence of large eigenvalues which allows to treat most of the terms explicitly. We closely follow the work of Bell et al. (2004) and extend it to multiphase problems. This novel method is validated by comparing results obtained with those of the fully explicit solver from the second and third chapters of this thesis.

1.3.3 Introduction of water film on bottom wall

In the fifth chapter of the thesis we describe a more realistic situation when gravity acts in the wall-normal direction. This force results in the movement of droplets towards the bottom wall where they merge and form a film of water. We model the film as a sufficiently thin layer neglecting internal motion and keeping it to a constant height. In order to maintain the height we add or drain water near the bottom wall. Simultaneously, we keep the total mass of water in the system constant on average by distributing new water droplets into the channel from the

top wall. We express the film temperature approximating it by a second order polynomial in the wall-normal coordinate (Russo et al. 2014b) and consider the film energy per unit area as dependent variable. The film is coupled to the carrier phase by evaporation and condensation of water vapor at its surface. The coupling between the film and the dispersed phase is through droplets merging with the film as they migrate downward due to gravity. In this chapter we analyze the behavior of droplets and the influence on the heat transfer due to the inclusion of the thin film.

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Chapter 2

Comparison of DNS of compressible and incompressible turbulent droplet-laden heated channel flow with phase transition

Abstract

Direct numerical simulation is used to assess the importance of compressibility in turbulent channel flow of a mixture of air and water vapor with dispersed water droplets. The dispersed phase is allowed to undergo phase transition, which leads to heat and mass transfer between the phases. We compare simulation results obtained with an incompressible formulation with those obtained for compressible flow at various low values of Mach number. We discuss differences in fluid flow, heat- and mass transfer and dispersed droplet properties. Results for flow properties such as mean velocity obtained with the compressible model converge quickly to the incompressible results in case the Mach number is reduced. In contrast, thermal properties such as the heat transfer, characterized by the Nusselt number, display a systematic difference between the two formulations on the order of 15%, even in the low-Mach limit. This shows the necessity of the use of a compressible formulation for accurate prediction of heat transfer, even in case of an initial relative humidity of 100%. Mass transfer properties display a difference between the models on the order of 5%, for example in the prediction of the droplet mean diameter near the walls.

2.1 Introduction

Multiphase flows with a large number of droplets dispersed into a gas play an important role in a variety of technological and environmental applications. Examples include thermal processing in food manufacturing, air pollution control and heat transfer in power stations (Barigou et al. 1998). In this paper we investigate a coupled Euler-Lagrange model to simulate droplet-laden turbulent channel flow in which phase transition plays an important role. We study in particular the effect of compressibility at low Mach numbers on the vapor and temperature fields and on the size distribution of the droplets. While the kinematics of the flow are found to be rather insensitive to compressibility at low Mach numbers, we observe a range of systematic differences in heat and mass transfer characteristics.

Not many studies focus on mass and heat transfer in droplet-laden turbulent flow. The first study was done by Mashayek in 1998. He conducted an Euler-Lagrange simulation study, investigating homogeneous turbulence with two-way coupling in momentum, mass and en-

ergy of the system. Later an overview of suitable techniques for the treatment of such type of problems was presented in Mashayek and Pandya (2003), and in Wang and Rutland (2006). Later, a study dedicated to the mixing layer with embedded evaporating droplets was conducted by Miller and Bellan (1998). In Masi et al. (2010) a cloud of inertial evaporating droplets, interacting with a non-isothermal droplet-laden turbulent planar jet, is considered. In the present paper we extend the work of Mashayek (1998) to wall-bounded turbulence by investigating turbulent channel flow with a dispersed droplet phase undergoing phase transition. All the studies mentioned above focus on evaporating droplets while in this study droplets may also grow by condensation of the vapor phase. To enable comparison between a strictly incompressible and a more general compressible formulation, we focus the attention on a case of initially 100% relative humidity in the channel. The models adopted here are identical to the models used in Miller and Bellan (1998) and Masi et al. (2010).

We study droplet-laden channel flow in which the top wall is heated uniformly and the bottom wall is cooled such that the total energy of the system is conserved. This leads to a temperature gradient in the wall-normal direction. As a point of reference we consider the flow of droplets of water in air, in which the presence of water vapor is accounted for. The mixture of air and water vapor will be referred to as the carrier phase or the carrier gas and liquid droplets as the dispersed phase. The system investigated in this study contains a rather small amount of water vapor, which motivates to approximate several transport characteristics of the carrier phase as those of clean air and investigate trends in flow and in heat and mass transfer properties due to the presence of vapor and liquid water droplets.

Incorporation of evaporation and condensation of the dispersed phase raises the question whether or not to include explicit compressibility of the carrier phase. If the carrier gas is assumed to be strictly incompressible then the inclusion of evaporation and condensation is subject to the condition that all instantaneous changes in the local mass density of air and water vapor cancel each other precisely throughout the domain. A full simulation model can be developed for such an incompressible carrier phase (Russo et al. 2014). Here, we confront the incompressible model with a fully compressible description, which allows to quantify the consequences of non-constant mass density of the carrier phase and indicates in which respects and under what conditions the full compressible formulation becomes essential.

We investigate the sensitivity of flow and transport characteristics arising from low-level compressibility effects in multiphase systems. For that purpose we analyze the results from simulations using two different approaches, i.e., a fully incompressible flow model and a compressible formulation. We compare thermal quantities of the system, such as the Nusselt number and mean temperature profiles, along with properties of the dispersed phase, such as accumulation of droplets near the walls and droplet size distribution history, in order to conclude for which quantities and flow conditions the compressible formulation should be used and for which other quantities the approximate incompressible model is adequate. Differences are deliberately kept small by focussing on an initial relative humidity of 100%; this helps to identify the sensitivity of resulting quantities to compressibility effects at low Mach numbers.

The organization of this paper is as follows. In Section 2.2 the mathematical model is formulated for the coupled droplet-carrier gas system. The numerical methods for both formulations are presented in Section 2.3. The initial conditions for the two models are described in Section 2.4. Finally, the results of the incompressible and compressible formulations regarding flow properties, heat and mass transfer and dispersed phase characteristics are presented in Section 2.5 and the concluding remarks are collected in Section 2.6.

2.2 The governing equations

This section is dedicated to the mathematical model. First, the geometry of the problem will be described along with the applied boundary conditions. Subsequently, the set of partial differential equations for the carrier phase, the system of ordinary differential equations for the dispersed phase and the source terms describing the coupling between the two phases will be presented in separate subsections. At the end of each subsection the differences between the equations used in the incompressible model (Russo et al. 2014) and in the current study will be emphasized.

2.2.1 The carrier phase

We consider a water-air system in a channel, bounded by two parallel horizontal plates. In Fig.2.1 a sketch of the domain is presented. The domain has a size of $4\pi H$ in the streamwise direction, which is denoted by x , and $2\pi H$ in the spanwise direction, z , where H is half the channel height. In addition, y is the coordinate in the wall-normal direction. The total volume of the domain is defined by V . The top wall of the channel is denoted by $y = H$ and the bottom wall by $y = -H$. Studies done by Kim et al. (1987) motivate us to use periodic boundary conditions in the streamwise and spanwise directions. In addition, no-slip conditions are enforced at the walls. A constant heat flux $\dot{Q}$ is applied through the walls: this heat flux is positive through the top wall and negative through the bottom wall. The flux at both walls is equal in size in order to conserve the total energy of the system. As a consequence, the gas temperature is higher near the top wall and lower near the bottom, and a gradient of temperature develops across the channel.

2.2.1.1 The compressible formulation

The carrier phase is treated as a compressible Newtonian fluid. We impose conservation of mass, momentum, total energy density and water vapor. The equations can be written as Mashayek (1998):

$$\partial_t \rho + \partial_j (\rho u_j) = Q_m \quad (2.1)$$

$$\partial_t (\rho u_i) + \partial_j (\rho u_i u_j) = -\partial_i p + \partial_j (\mu(T) S_{ij}) + F_i + Q_{mom,i} \quad (2.2)$$

$$\partial_t e + \partial_j ((e + p) u_j) = \partial_j (K(T) \partial_j T) + \partial_j (u_i \mu(T) S_{ij}) + \quad (2.3)$$

$$\begin{aligned} & \partial_j (\rho D \partial_j Y_v ((c_{pv} - c_{pa}) T + \lambda)) + Q_e \\ & \partial_t (\rho Y_v) + \partial_j (u_j \rho Y_v) = \partial_j (\rho D \partial_j Y_v) + Q_m \end{aligned} \quad (2.4)$$

This system is solved for mass density ρ , velocity components u_i , total energy density e and vapor mass fraction Y_v . The source terms Q_m , $Q_{mom,i}$, Q_e express the interaction between the phases and will be described in detail in subsection 2.2.3. The term F_i is an external force density. Applying periodic boundary conditions in the streamwise direction, we have to make

a choice for the calculation of this forcing term in order to maintain the flow in the channel. In the current study it is chosen in such a way that the total momentum in the streamwise direction is constant in time.

In our model ρ and ρY_v denote the mass density of the carrier gas and water vapor in the considered volume, respectively. At the same time the carrier phase is composed of pure air and water vapor:

$$\rho = \rho_{air} + \rho_{vapor} \quad (2.5)$$

In equations (2.1) and (2.4) the same mass source term Q_m appears. This term reflects the change in mass of the carrier gas and water vapor because of evaporation and condensation. Since only vapor can contribute to the change of mass density of the carrier phase through phase transitions, equations (2.1) and (2.4) have the same coupling term.

The pressure p is defined through the ideal gas law for a two-component mixture in the following way (Miller and Bellan 1998):

$$p = \rho T R_{air}(1 - Y_v) + \rho T R_{water} Y_v \quad (2.6)$$

where T denotes the temperature of the carrier gas. In addition, R_{air} and R_{water} stand for the specific gas constants for air and water vapor, respectively. They are equal to the universal gas constant, divided by the corresponding molar mass. In equation (2.2) S_{ij} is the compressible extension of the rate-of-strain tensor defined as $S_{ij} = \partial_i u_j + \partial_j u_i - \frac{2}{3} \Delta \delta_{ij}$ where $\Delta = \partial_k u_k$ denotes the divergence of the velocity. Here and elsewhere we adopt the summation convention implying summation over repeated indices.

The dynamic viscosity of the carrier gas μ depends on temperature through Sutherland's law (Sutherland 1893), i.e.:

$$\mu = \mu_{ref} \left(\frac{T}{T_{ref}} \right)^{\frac{3}{2}} \frac{T_{ref} + S}{T + S} \quad (2.7)$$

where μ_{ref} is the dynamic viscosity of air at the reference temperature T_{ref} . In addition, S is the Sutherland temperature and for the case of air $S = 110.4$ K. In (2.7) the presence of water vapor in the carrier phase is not taken into account since the mixture air - water vapor considered here is assumed to have a sufficiently small vapor mass fraction.

In equation (2.3) K stands for the thermal conductivity of the carrier gas which depends on temperature such that ratio of K and μ is constant (Bird et al. 1960). In addition, D in (2.4) denotes the diffusion coefficient of water vapor in air, which also depends on temperature such that ratio $\rho D / \mu$ is constant (Bird et al. 1960).

The total energy density of the fluid e is the sum of the kinetic energy density and the internal energy density, i.e., $e = e_{int} + e_{kin}$, where (Miller and Bellan 1998)

$$e_{kin} = \frac{1}{2} \rho u_j u_j \quad (2.8)$$

$$e_{int} = \rho c_{va} T (1 - Y_v) + \rho c_{vv} T Y_v + \rho \lambda Y_v \quad (2.9)$$

Here c_{va}, c_{vv} are the values of the specific heats at constant volume of air and water vapor and λ is the latent heat. Likewise, c_{pv} and c_{pa} in equation (2.3) denote the specific heats at constant pressure of water vapor and air, respectively. The first term on the right-hand side of equation (2.9) is the internal energy density of air while the two other terms denote the

internal energy density of the vapor contained in the carrier phase. Gas temperature T is calculated from the total energy density e using (2.8) and (2.9).

The system of governing equations (2.1)-(2.4) is made non-dimensional using a set of reference scales of the system. The reference temperature, T_{ref} , is the initial mean temperature of each test case, while the reference mass density, ρ_{ref} , is the initial mean mass density of the carrier gas. The reference length L_{ref} is chosen as half the channel height H ; specifically, we consider a water-air system flowing between a channel with $L_{ref} = 2$ cm. The velocity scale u_{ref} is taken as the bulk velocity u_b of the carrier gas. The Reynolds number based on the reference scales is defined in the following way:

$$Re_b = \frac{\rho_{ref} u_b L_{ref}}{\mu(T_{ref})} \quad (2.10)$$

where $\mu(T_{ref})$ is the dynamic viscosity of air at T_{ref} . As a result of making the governing equations non-dimensional, the final system of equations also contains the Prandtl number Pr , the Mach number Ma and the Schmidt number Sc . Pr is the ratio of kinematic viscosity to thermal diffusivity:

$$Pr = \frac{c_{pa} \mu(T_{ref})}{K(T_{ref})} \quad (2.11)$$

The Mach number expresses the ratio of the reference velocity to the speed of sound at T_{ref} ; $Ma = u_{ref}/c(T_{ref})$ where $c(T_{ref})$ is the reference speed of sound. The speed of sound is calculated using the assumption of a sufficiently small amount of water vapor in the carrier gas, and the ideal gas law:

$$c(T) = \sqrt{\frac{\gamma_{air} R T}{M_{air}}} \quad (2.12)$$

where γ_{air} is defined as the ratio between the specific heats at constant pressure and constant volume of air, equal to 1.4. In addition, M_{air} is the molar mass of air, $M_{air} = 0.0289645$ kg/mol. The Schmidt number Sc denotes the ratio of kinematic viscosity to mass diffusivity:

$$Sc = \frac{\mu(T_{ref})}{\rho_{ref} D(T_{ref})} \quad (2.13)$$

We take into account the dependence of viscosity on temperature (2.7) and assume specific heats to be constant. The temperature dependence of the thermal conductivity K and diffusion coefficient D can hence be inferred. The values of the main thermal quantities are shown for different T_{ref} used in this paper in Table 2.1. The Reynolds number is determined by specifying the mass flow rate - the selected value of Re_b corresponds to values of the friction Reynolds number Re_τ about 150, a well-documented case of turbulent channel flow in literature (Marchioli et al. (2008)). Throughout, we will fully adhere to the values of Re_b , Sc and Pr . The value of Ma is too low to allow full simulations, including the gathering of converged statistics, with the current numerical method. Instead, we will relax the requirement on Ma and choose low, but considerably higher values of 0.05, 0.1 and 0.2 to investigate the trends. Simulation times of 8-10 months are required on 32 CPU's of a modern supercomputer at

$Ma = 0.05$. Infeasible requirements on available computing budgets would be required for $Ma = 0.005$. Conversely, as this study will show, much, if not all, of the flow physics and heat and mass transfer characteristics can accurately be approximated using Ma in the selected range. Current research into tailored low-Mach time-stepping algorithms that would allow simulation at the physical Ma is ongoing and will be presented elsewhere.

Fig. 2.1: : The computational domain

T_{ref} (K)	293.15	323.15
K (W/m · K)	2.5519×10^{-2}	2.7889×10^{-2}
μ (kg/m · s)	1.86766×10^{-5}	2.012×10^{-5}
D (m ² /s)	2.0917×10^{-5}	2.4244×10^{-5}
ρ_{ref} (kg/m ³)	1.194	1.0426
u_b (m/s)	1.8246	2.25104
c (m/s)	343.111	360.2403
c_{pa} (J/kgK)	1010	1010
Re_b	2333	2333
Pr	0.7478	0.7959
Ma	0.00532	0.00625
Sc	0.6283	0.6505

Table 2.1: Parameters of the flow depending on the reference temperature

2.2.1.2 The incompressible formulation

It is known that for values of the Mach number up to 0.3 the fluid mechanics of turbulent channel flow corresponds well to that of incompressible flow (Anderson 2007). There are three main differences between compressible and incompressible flows: a constant mass density, a zero divergence of the velocity and an infinite speed of sound in incompressible flow. The incompressible formulation for the carrier phase adopted by Russo et al. (2014) implies that evaporation and condensation are subject to the condition that all instantaneous changes in the local mass density of air and water vapor cancel each other precisely throughout the domain. This is required to maintain a constant mass density of the carrier phase. In fact, $\rho = \rho_{air}(\mathbf{x}, t) + \rho_{vapor}(\mathbf{x}, t)$ where mass densities are functions of position and time. Consequently, we have the following:

$$\nabla \rho_{air} = -\nabla \rho_{vapor}, \quad \partial_t \rho_{air} = -\partial_t \rho_{vapor} \quad (2.14)$$

which is an unphysical constraint, inherent to the incompressible formulation.

The incompressible treatment of the carrier phase still permits to incorporate changes in mass density into the model using the equation of state and the Boussinesq approximation, which implies the dependence of mass density on temperature and vapor mass fraction. In our problem the divergence of velocity is not equal to zero because of phase transitions. Apart from this, the heat flux in the considered problem leads to a net transfer of gas from the hot to the cold wall during the initial stages during which the mean temperature gradient in the wall-normal direction develops. This will be discussed in more detail in section 2.5.

Apart from the assumption that the flow is incompressible, the treatment of pressure makes the two formulations different. While an explicit equation of state is used to connect pressure and temperature in the compressible case, the incompressible formulation solves the pressure from a Poisson equation derived from the condition of a divergence-free velocity field.

Another difference in the governing equations for the carrier phase is due to the viscous dissipation term. While it is present through the term $\partial_j(u_i \mu(T) S_{ij})$ in the total energy density equation in the compressible formulation, it is absent in the temperature equation in the incompressible formulation. This term is expected to have only a small influence on the results as will be discussed in Section 2.5.

In addition, there are also some differences in the physical modeling used in the two approaches. In the compressible formulation we incorporate the dependence of the dynamic viscosity μ on the temperature of the carrier phase through Sutherland's law. In the incompressible formulation μ is kept constant. Moreover, in the compressible approach K depends on temperature such that the ratio of K and μ is constant. In this formulation we do not consider the thermal conductivity of a mixture since vapor mass fractions are typically small. In the incompressible approach the thermal conductivity of a mixture is incorporated, however, thermal conductivities of water vapor and pure air are considered constant and not dependent on temperature. In addition, the thermal diffusivity D depends on temperature in the compressible formulation such that the ratio $\frac{\rho D}{\mu}$ is constant, while in the incompressible formulation D is considered constant. All these are small differences: the typical mass fraction of water vapor contributes on the order of 1% to the mass density of the carrier phase, and the variations in temperature throughout the domain are on the order of 1 – 2% in the test cases considered. We performed a simulation with exactly the same model for the carrier gas in the compressible formulation as used in the incompressible. The found differences in gas and

droplet quantities are on the order of 0.001% of the mean values. As a consequence, these small differences between the models do not appreciably influence the level of agreement between the two formulations.

In this study we will compare results from the incompressible carrier phase with those obtained using a varying mass-density of the carrier gas in the compressible formulation. As a result we may then also appreciate under which physical circumstances the compressible formulation deviates significantly from the incompressible model.

2.2.2 Equations for droplets

The dispersed phase of the system consists of droplets which are distributed over the total volume of the channel. They are assumed to collide elastically with the solid walls. In these collisions no heat is transferred. Periodic boundary conditions are applied to the droplets: if a droplet leaves the domain, it is reinserted at the opposite boundary with the same properties. Referring to the classification proposed by Elghobashi (1994), we focus on droplet volume fractions high enough so that two-way coupling is required, while the volume fraction is low enough for the effects of collisions between droplets to be negligible. This regime corresponds to droplet volume fractions from 10^{-6} to 10^{-3} . In the current study the droplet volume fraction fluctuates around 10^{-4} .

For both the compressible and the incompressible model the same system of ordinary differential equations for the dispersed phase is adopted and this will be discussed in detail in this subsection. The model for the dispersed phase uses a point-particle approach. We assume that the droplets are spherical and include evaporation and condensation to describe the response of the droplets to the thermodynamic conditions found in the carrier gas along their trajectories.

The droplets are tracked individually in a Lagrangian manner. We solve a system of ordinary differential equations for position, velocity, temperature and mass of each droplet. The location of a droplet is governed by the kinematic condition:

$$\frac{d\mathbf{x}_i(t)}{dt} = \mathbf{v}_i \quad (2.15)$$

where $\mathbf{x}_i$ is the location and $\mathbf{v}_i$ is the velocity of droplet i .

For the water-air system droplets have a much higher mass density than the carrier fluid. The Stokes drag force is the dominant force in these circumstances (Armenio and Fiorotto 2001). We do not consider gravity acting on the droplets in the current study and solve the equation of motion for each droplet:

$$\frac{dm_i \mathbf{v}_i}{dt} = m_i \frac{\mathbf{u}(\mathbf{x}_i, t) - \mathbf{v}_i}{\tau_{d,i}} \left(1 + 0.15 \text{Re}_{d,i}^{0.687} \right) + \mathbf{v}(\mathbf{x}_i, t) \frac{dm_i}{dt} \quad (2.16)$$

where m_i is its mass and $\mathbf{u}(\mathbf{x}_i, t)$ is the velocity of the carrier gas at the droplet position. In addition, we define $\text{Re}_{d,i}$ as the Reynolds number based on the diameter d_i of the droplet and on the relative velocity, $\text{Re}_{d,i} = d_i \rho |\mathbf{u}(\mathbf{x}_i, t) - \mathbf{v}| / \mu$. Moreover, $\tau_{d,i} = \rho_l d_i^2 / (18\mu)$ defines the droplet relaxation time which quantifies how fast a droplet adjusts its motion to the local

flow. The first term on the right-hand side in (2.16) is the drag force for which the Schiller-Naumann correlation is used (Schiller and Naumann 1933). This correlation was reported accurate for $Re_{d,i}$ between 0 and 1000, which range of conditions is fully adequate for our simulations. The second term on the right-hand side of (2.16) reflects the contribution from the momentum of the vapor in case of evaporation or condensation of water vapor. The vapor has the same velocity as the droplet at the moment it condenses or it has just been evaporated at the droplet surface.

In this study we do not consider nucleation of droplets. In fact, homogeneous nucleation only occurs when the relative humidity is significantly larger than 100%, which in the current study does not occur.

In the current study the assumption of a uniform temperature inside a droplet is used. This can be motivated by the Biot number which is the ratio of the heat transfer resistance inside the droplet to the heat transfer resistance at the surface of the droplet, $Bi = h_m d_i / k_d$ where h_m and k_d denote the convective heat transfer coefficient from gas to droplet and the droplet thermal conductivity, respectively. This dimensionless number determines whether the temperature varies significantly within the droplet. One may expect an almost uniform temperature to good approximation if $Bi \ll 1$ (DeWitt et al. 2007). In the current study we use the following correlation for h_m for small droplets, valid for low values of $Re_{d,i}$ (Bird et al. 1960):

$$\frac{h_m d_i}{K} = 2 + 0.6 Re_{d,i}^{1/2} Pr^{1/3} \quad (2.17)$$

In actual simulations we found that the pdf of $Re_{d,i}$ contains most of its statistical mass in the range $Re_{d,i} \leq 1$, with some low-probability events up to $Re_{d,i} = 5$. The values of $Re_{d,i}$ are contained in such narrow range in these simulations since gravity was not included. The resulting Biot number is therefore only slightly higher than the ratio of the thermal conductivity of the carrier gas and the droplet, $Bi = K/k_d = 0.046$; this motivates the assumption of a uniform temperature, T_i , inside a droplet.

The total energy of droplet i is given by $E_i = \frac{1}{2} m_i |\mathbf{v}_i|^2 + c_l m_i T_i$, where c_l is the specific heat of liquid water. This energy may change because of two mechanisms: (i) condensation and evaporation and (ii) the heat exchange by convection at the droplet surface which arises due to the temperature difference between the surroundings and the droplet surface:

$$\frac{d}{dt} E_i = h_v \frac{dm_i}{dt} + h_m A_i (T(\mathbf{x}_i, t) - T_i) \quad (2.18)$$

For the convective contribution, we will use the correlation for forced convection around a sphere (Bird et al. 1960) under the assumptions of uniform surface temperature and small net mass-transfer rate. Under these circumstances we can adopt the expression for the heat transfer coefficient h_m as in (2.17). In addition, A_i in the convective term denotes the surface area of the droplet.

The first contribution on the right-hand side of (2.18) contains the specific enthalpy of vapor, where

$$h_v = \lambda_0 + c_{pv} T_i \quad (2.19)$$

Here λ_0 stands for the latent heat at temperature equal to 0 K and c_{pv} denotes the specific heat at constant pressure of water vapor.

In order to close the system of equations we require an expression for dm_i/dt , the rate of evaporation and condensation of a droplet. Assuming a vapor film around the droplets of uniform width δ , we may use the following equation for the change of the droplet mass, m_i (Bird et al. 1960):

$$\frac{dm_i}{dt} = -\frac{m_i \text{Sh}}{3\tau_{d,i} \text{Sc}} \ln \left(\frac{1 - Y_{v,\delta,i}}{1 - Y_{v,s,i}} \right) \quad (2.20)$$

where $Y_{v,\delta}$ and $Y_{v,s}$ are the vapor mass fractions at a distance δ from the surface of the droplet and on the surface of the droplet, respectively. Here, we adopted the Schmidt number $\text{Sc} = \mu/(\rho_l D)$ and the Sherwood number $\text{Sh} = d_i/\delta$ (Bird et al. 1960). In addition, for the Sherwood number we use the correlation for a sphere (Bird et al. 1960):

$$\text{Sh} = 2 + 0.6\text{Re}_d^{1/2} \text{Sc}^{1/3} \quad (2.21)$$

The driving quantity in (2.20) is the difference $Y_{v,\delta,i} - Y_{v,s,i}$. The vapor mass fraction at the surface, $Y_{v,s}$ corresponds to thermodynamic equilibrium at the surface, which determines the saturation vapor pressure. The saturation pressure $p_{v,sat}$ is calculated using Antoine's relation (Antoine 1888):

$$p_{v,sat} = 10^5 \exp \left(A - \frac{B}{C + T_i} \right) \quad \text{in Pa} \quad (2.22)$$

where $A = 11.6834$, $B = 4089.59 \text{ K}$ and $C = 500.02 \text{ K}$. Subsequently, the ideal gas law for water vapor is used to calculate the vapor mass fraction at the surface of the droplet:

$$Y_{v,s,i} = \frac{p_{v,sat}(T_i)}{\rho R_{water} T_i} \quad (2.23)$$

In order to find $Y_{v,\delta,i}$, i.e., the vapor fraction in the close vicinity of the droplet, the assumption of a point-particle approach motivates to calculate $Y_{v,\delta,i}$ as the vapor mass fraction of the carrier gas at the position of the droplet, i.e., $Y_{v,\delta,i} = Y_v(\mathbf{x}_i, t)$.

2.2.3 Coupling terms

The governing equations for the carrier phase contain two-way coupling terms. These terms appear because of the mass, momentum and energy exchange between the carrier and the dispersed phases. The interaction between the two phases conserves mass, momentum and energy. The contributions from the dispersed phase in the equations of mass, momentum, energy and water vapor for the carrier gas are given by:

$$Q_m = -\sum_i \frac{dm_i}{dt} \delta(\mathbf{x} - \mathbf{x}_i) \quad (2.24)$$

$$\mathbf{Q}_{mom} = -\sum_i \frac{d}{dt} (m_i \mathbf{v}_i) \delta(\mathbf{x} - \mathbf{x}_i) \quad (2.25)$$

$$Q_e = - \sum_i \frac{d}{dt} \left(c_l m_i T_i + \frac{1}{2} m_i |\mathbf{v}_i|^2 \right) \delta(\mathbf{x} - \mathbf{x}_i) \quad (2.26)$$

where the sums are taken over all droplets in the domain. The delta-function expresses that the coupling terms act only at the positions of the droplets, consistent with the underlying point-particle assumption.

The coupling term (2.24) in the mass density equation shows that mass transfer between the phases occurs because of evaporation and condensation. In order to calculate this term equation (2.20) will be used. Momentum transfer between the phases as expressed by (2.25), consists of two mechanisms: the drag force between the droplets and the carrier gas and the momentum transfer due to mass transfer arising from phase changes. In order to calculate this coupling term equation (2.16) will be used, rewritten to provide $d(m_i v_i)/dt$ as required. Finally, in (2.26) the first term on the right-hand side represents the convective heat transfer and the energy transferred to the carrier phase by vapor. The last term in (2.26) appears as the contribution from the kinetic energy of the droplets. This contribution can be evaluated from the right-hand side of (2.18).

This completes the description of the governing equations for the two phases. In the next section we will describe the numerical approaches used for the treatment of the governing equations for the two phases and the coupling terms.

2.3 Numerical method

In this section the numerical approaches applied to the compressible and incompressible formulations will be described. In addition, the numerical methods for the dispersed phase and implementation of the coupling terms will be discussed.

The incompressible and compressible models are simulated using different numerical methods. The incompressible formulation adopts a pseudo-spectral method for the carrier phase as described in Russo et al. (2014) and Kuerten (2006). In the two periodic directions, x and z , a Fourier-Galerkin approach is used, while a Chebyshev-collocation approach is applied in the wall-normal direction, y . The droplet equations are integrated in time with the same three-stage Runge-Kutta method as used for the convective terms in the carrier phase equations. The viscous terms and pressure are integrated in time with the implicit Crank-Nicolson method. The pressure is found at each time level from the divergence-free condition for the velocity, following the approach proposed by Kleiser and Schumann (1980).

The numerical model for the compressible carrier phase adopts a second-order accurate explicit four-stage low-storage Runge-Kutta time-stepping with weights equal to $1/4$; $1/3$; $1/2$ and 1 . A second order finite volume discretization (Vreman et al. (1992)) is used. The geometry is divided into rectangular cells. A uniform grid is used in the two periodic directions. The grid spacing is denoted by Δx and Δz for the streamwise and the spanwise direction, respectively. In the wall-normal direction a non-uniform grid is applied which is finer near the walls. We use 128 grid points in each direction. This choice for the grid resolution is motivated in detail in Marchioli et al. (2008) where simulation results obtained with various numerical methods were compared. In fact, simulation of a particle-laden turbulent channel flow at $Re_\tau = 150$ using second-order central differences, similar to our method, on the same grid as used here were reported. The results of this simulation showed a good agreement in

gas and particle statistics with other studies based on pseudo-spectral methods. In fact, an agreement on the order of 1% in the mean velocity profile and on the order of 2% in RMS of fluctuating quantities was observed. This demonstrates the reliability of the DNS results reported in this paper and shows that the basic mechanisms are captured well enough to distinguish compressibility effects in multiphase flows.

The variables are stored in the centers of the cells. For each of the cells we integrate the governing equations (2.1) - (2.4) for the carrier phase in conservative form over the volume of the cell. For the integrals of the coupling terms we proceed as follows. As an example, we consider the integration over a grid cell of the coupling term for the mass density equation. Substituting the explicit expression for it, (2.24), we obtain:

$$\int_{V_{cell}} Q_m dV = - \sum_i \int_{V_{cell}} \frac{dm_i}{dt} \delta(\mathbf{x} - \mathbf{x}_i) dV = - \sum_{i \in cell} \frac{dm_i}{dt}(\mathbf{x}_i) \quad (2.27)$$

where the last sum is taken over all droplets within the cell. At any time, a droplet contributes only to the flux in the grid cell where it is located. The size of the droplet is everywhere smaller than the smallest grid size. The smallest grid size in wall units is equal to 0.6 while the droplet diameter in wall units equals to 0.5.

The system of ordinary differential equations for the droplets is integrated in time applying the same four-stage compact Runge-Kutta method as used for the gas equations. The right-hand sides of the droplet equations contain gas properties at droplet location. In order to determine these, tri-linear interpolation is applied (Marchioli et al. 2008).

2.4 Initial conditions of the simulations

In this section the initial conditions for the different test cases will be described and motivated, both for the compressible and the incompressible formulations.

In this study two sets of simulations are chosen. The first set considers applying three different values of the Mach number, 0.2, 0.1 and 0.05 to a system under atmospheric pressure and room temperature. We will study convergence of the results to the incompressible results when decreasing the Mach number. The value of the Mach number based on the reference conditions is about 5×10^{-3} . A Mach number this small leads to a further reduction of the time step for the chosen explicit numerical method, which would render the simulations infeasible.

In all the cases the simulations were started from a turbulent velocity field, obtained from a simulation without droplets at the correct values of the Mach number and the Prandtl number. These simulations were done with adiabatic boundary conditions at the walls until the statistically steady state was reached. The resulting temperature profiles are shown in Figure 2.2 for the three different values of the Mach number as well as for the incompressible case for which the initial temperature is uniform. The initial mean temperature for these simulations was chosen equal to 293.15 K. The highest Mach number leads to variations in temperature on the order of 1%. It is seen that reduced compressibility implies that the initial conditions for the compressible cases converge to those of incompressible flow.

We apply the condition of uniform relative humidity within the channel in all cases. Rela-

tive humidity ϕ characterizes the amount of vapor in the channel. It is the ratio of the partial pressure p_v of water vapor in the air-vapor mixture to the saturated vapor pressure at the prescribed temperature, $\phi = p_v/p_{v,sat}$. The condition of $\phi = 100\%$ was selected in order to have very ‘mild’ coupling conditions for the turbulent flow in the channel as far as mass transfer is concerned, resulting in the smallest differences between the compressible and the incompressible formulations. From the state equation for water vapor we find the vapor mass fraction in the channel:

$$Y_v = \frac{p_{v,sat}(T_{ref})}{\rho R_{water} T_{ref}} \quad (2.28)$$

where $p_{v,sat}(T)$ follows from (2.22). Subsequently, the total energy density is found taking into account the contribution from the added water vapor according to (2.9).

We randomly distribute $N_{drop} = 2,000,000$ identical droplets over the volume of the channel and apply a positive heat flux at the top wall and a negative flux of equal magnitude at the bottom wall. For both the incompressible and the compressible simulations the initial droplet diameter is given by $d_i/H = 3.09 \times 10^{-3}$. In this way, the initial volume fraction of droplets is on the order of 10^{-4} . The Kolmogorov length varies along the wall-normal direction from a minimum value of 1.6 near the wall to a maximum value of 3.6 in wall units at the centerline (Marchioli et al. (2008)). Consequently, the maximum ratio of the droplet diameter, which is in wall units equals to 0.5, and the Kolmogorov scale is equal to approximately 0.3. This ratio shows that it is allowed to use the point-particle approach, (Marchioli et al. (2006)), (Elghobashi (1994)). Velocity and temperature of the droplets are initialized using the carrier gas values at the droplet locations.

The second set of simulations reflects physical situations at $\phi = 100\%$ for which the effect of compressibility is expected to be more important. We will investigate the effects of a higher heat flux through the walls and a higher mean temperature. In the first case we will apply a five times larger heat flux through the walls and in the second the mean temperature will be increased to 323.15 K. Both these changes are quite significant while keeping the flow and process regime comparable, e.g., not inducing effects of boiling. A description of all test cases can be found in Table 2.2.

The slightly higher heat flux in case 5 of about 9% is chosen in order to obtain the same temperature gradient at the walls as in cases 1-3, compensating for the temperature dependence of the thermal conductivity of the carrier gas, which, according to Table 2.1 changes by the same amount. In the next section we will discuss the results obtained from these two sets of simulations.

case number	Ma	$\dot{Q}$ (W/m ²)	T_{mean} (K)
1	0.2	31.8987	293.15
2	0.1	31.8987	293.15
3	0.05	31.8987	293.15
4	0.05	159.49	293.15
5	0.05	34.8612	323.15

Table 2.2: The carrier gas conditions for the compressible simulations

Fig. 2.2: : Initial fluid temperature averaged over the homogeneous directions as a function of the wall-normal coordinate; dashed: incompressible, circles: $Ma = 0.2$; dash-dotted: $Ma = 0.1$; solid: $Ma = 0.05$.

2.5 Results

In this section the results obtained with the compressible and incompressible formulations will be compared. The main purpose of the comparison is to see whether and which compressible results converge to the incompressible results if we decrease the value of the Mach number. We concentrate on fluid flow aspects, heat transfer properties of the system and on the behavior of the droplets and adopt a spatial resolution of $128 \times 128 \times 128$ with both the finite volume and the spectral method. Four subsections will be presented: in 2.5.1 the agreement in the kinematics of the flow between the two formulations is shown, 2.5.2 is dedicated to thermal properties of the carrier phase, in 2.5.3 results for the water vapor are presented and finally, in 2.5.4 we present results of the dispersed phase.

2.5.1 Velocity properties

In this study we investigate compressibility in the form of changes in the mass density due to phase transition taking liquid water from the dispersed water droplets to the vapor and vice versa. This compressibility is expressed by a non-zero divergence of velocity and a non-zero gradient of the mass density. In order to quantify this explicit compressibility we compared the RMS of the term $\rho \nabla \cdot \mathbf{u}$ with the RMS of the term $\mathbf{u} \cdot \nabla \rho$ in the continuity equation. In Figure 2.3 we display these as functions of the wall-normal coordinate. We observed that both during the initial stages of the simulations as well as in a well developed stage the RMS of these two terms is of the same order of magnitude, accounting for changes in the local density on the order of a few percent. At initial conditions with stronger heat flux and higher

mean system temperature these explicit compressibility effects are more pronounced. First, we establish the level of agreement in the kinematics of the turbulent flow in both formulations. In Figure 2.4a the streamwise component of the carrier gas velocity averaged over the periodic directions and over time is presented. The maximum difference between the two formulations at $Ma = 0.2$ is on the order of 2%. In addition, the bulk Reynolds number history as defined in (2.10) is presented in Figure 2.4b. The difference is on the order of 1%. For both formulations the bulk Reynolds number increases in time. The forcing of the flow is chosen in such a way that the total momentum of the system, the sum of the momentum of the carrier and dispersed phases, is conserved. Droplets tend to migrate to the walls (see section 2.5.4), where they will gradually obtain a lower streamwise velocity. That implies that the carrier gas will gain momentum and this causes the gradual increase of the bulk Reynolds number. At reduced Ma the correspondence between the two formulations becomes even closer and the maximum difference in the averaged streamwise velocity is about 1% at $Ma = 0.1$ and $Ma = 0.05$. This also establishes the level of correspondence between the two independent direct numerical simulations at a resolution of 128^3 , employing very different numerical methods for spatial discretization as well as time integration.

Fig. 2.3: Solid: RMS of $\rho \nabla \cdot \mathbf{u}$, dashed: RMS of $\mathbf{u} \cdot \nabla \rho$ as a function of the wall-normal coordinate. (a): at 0.02s , (b): at 4s .

2.5.2 Heat transfer properties

We apply a heat flux to the walls, which induces a temperature gradient in the wall-normal direction: a region with higher temperatures forms near the warmer top wall and a region with lower temperatures near the colder bottom wall. During the initial transient period the carrier phase adapts to the applied boundary conditions and an asymmetric profile of the gas temperature develops from the initial nonuniform temperature field, cf. Figure 2.2. The evolution of the profile of the mean temperature, averaged over the homogeneous directions, is

Fig. 2.4: (a) Streamwise velocity component averaged over the homogeneous directions and over time $[2s; 8s]$ as a function of the wall-normal coordinate. (b): The bulk Reynolds number history. Compressible simulations (solid lines) are obtained at $Ma = 0.2$, incompressible model is shown with dashed lines, following the settings of Case 1.

presented in Figure 2.5 for two different values of the Mach number. It is seen that reduced compressibility implies a more symmetric profile of the mean temperature at later times.

In Figure 2.6 the asymptotic mean temperature profile is presented for different values of the Mach number and for the incompressible formulation. The carrier gas reaches a statistically steady state for which the mean temperature profiles can be determined after approximately $2s$. The results are averaged over time interval $[2s; 8s]$ and over the homogeneous directions. From figure 2.6 it can be concluded that a reduced compressibility in the compressible formulation leads to a strongly increased agreement with the results obtained with the incompressible model. Averaging over a longer time interval does not change the conclusions.

In Figure 2.6 one can observe significant differences between the temperature profiles for $Ma = 0.2$ and for $Ma = 0.05$. These differences are characteristic for the superposition of two effects. On the one hand, in the statistically steady state the adiabatic simulations yield a non-uniform temperature profile. For the larger Mach number the temperature profile is more non-uniform while remaining symmetric. This reflects the property that not the mean temperature is constant in compressible turbulent channel flow, but rather the stagnation temperature. On the other hand, the application of the heat flux to the walls at $Ma = 0$ leads to an anti-symmetric temperature profile. Combined, the symmetric (no heat flux) and anti-symmetric ($Ma = 0$) profiles lead to the characteristic profile shown. This superposition is present at all Mach numbers, but at $Ma = 0.2$ both effects are of the same magnitude, explaining the apparent qualitative difference.

Figure 2.7a shows how the root-mean square of the gas temperature evolves at $Ma = 0.2$. The maximum value of oscillations is equal to approximately 0.4 K which is around 10% of the temperature difference between the two walls.

Figure 2.7b shows the agreement of the root-mean square of the gas temperature for the incompressible and compressible formulations. It can be seen that the agreement between the two formulations increases if the Mach number is reduced. The level of variation in T_{rms} at

low Mach numbers, compared to the incompressible results is expected to represent slight differences resulting from differences in the numerical methods at the selected spatial resolution - currently, further grid refinement is not feasible.

To express the efficiency of the heat transfer between the channel walls we consider the Nusselt number. It has been shown that the Nusselt number can be increased by more than a factor of two if solid particles with high heat capacity are added to a turbulent channel flow (Kuerten et al. 2011). The Nusselt number is defined in the following way:

$$\text{Nu} = \left(\frac{d\bar{T}_g}{dy} \Big|_{\text{wall}} \right) / \frac{\Delta\bar{T}_g}{2H} \quad (2.29)$$

where bars denote averaging over the two homogeneous directions, $\Delta\bar{T}_g$ is the difference in gas temperature between the two walls and the derivative with respect to the wall-normal coordinate in the numerator is the average over both walls. Figure 2.8a shows how the Nusselt number depends on time for both formulations. We observe a close agreement with a relative difference of up to about 10%. The compressible formulation predicts a slightly higher value than the incompressible model.

In the initial phase of the simulations the compressible and incompressible formulation result in differences in the value of the Nusselt number up to 3. Kuerten et al. (2011) showed that for incompressible flow with solid particles three contributions to the Nusselt number can be distinguished:

$$\text{Nu} = \text{Nu}_{\text{lam}} + \text{Nu}_{\text{turb}} + \text{Nu}_{\text{part}} \quad (2.30)$$

which correspond to the Nusselt number for laminar flow, a contribution from turbulence and a contribution from particles. For turbulent flow with droplets there are some additional contributions, but they can be shown to be negligible (Russo et al. 2014b). An important difference between compressible and incompressible flow is that Nu_{turb} in compressible flow can be written as:

$$\text{Nu}_{\text{turb}} = - - \frac{1}{\alpha\Delta\bar{T}} \int_{-H}^H \overline{u_2 T} \quad (2.31)$$

can be written as:

$$\text{Nu}_{\text{turb}} = - \frac{1}{\alpha\Delta\bar{T}} \int_{-H}^H \overline{u_2' T'} - \frac{1}{\alpha\Delta\bar{T}} \int_{-H}^H \overline{u_2 \bar{T}} \quad (2.32)$$

where $\bar{\cdot}$ means averaging over the periodic directions and α is the thermal diffusivity. For incompressible flow the second contribution in (2.32) is equal to zero, because the mean of the wall-normal component of the velocity equals zero in incompressible channel flow. Our simulation results for the compressible formulation show that this contribution of the mean wall-normal velocity component is larger than the other contribution by a factor of 3 in the initial phase of case 3. This explains the initial difference in Nusselt number shown in Figure 2.8a. The presence of the additional term in Nu_{turb} in the compressible formulation reflects the additional net transfer of the gas from the hot wall to the cold wall during the initial stages which increases the value of the Nusselt number.

Figure 2.8b shows the results of the two formulations for cases 3, 4 and 5. The Nusselt number obtained from the compressible simulations is slightly higher than the corresponding incom-

pressible result for all three cases considered. The case with the higher mean temperature gives a significant increase in the value of the Nusselt number by more than a factor of 2. This is related to the difference in mean temperature between the two walls, figure 2.9. In case 5 the temperature difference between the two walls is smaller by more than a factor of two than in case 3. In the statistically steady state of cases 3 and 5 the droplets near the walls have the same diameter, see Section 2.5.4, but in the case of a higher mean temperature the mass transfer rate from the droplets to the carrier gas is higher (Russo et al. 2014), adding correspondingly to the transfer of heat. This explains the higher Nusselt number in case 5. Figure 2.8b shows that the compressible formulation becomes more important in case 5. The results for case 3 and 4 show very close agreement - the solid lines and square-marked lines practically coincide in Figure 2.8b. The independence of the Nusselt number on the value of the applied heat flux is further illustrated by the temperature difference between the walls: this difference is approximately 5 times larger in case 4 than in case 3, Figure 2.9. Thereby the increase of the heat flux through the walls by a factor 5 is almost completely compensated by the same factor of increase in the temperature difference, hence leading to a nearly unchanged Nu in case 4, compared to the reference case 3.

We also performed simulations with the two codes for the case of solid particles and compared the agreement in the Nusselt number history for these simulations with the case of droplets, for case 5 of 323.15 K mean temperature. In case of particles dispersed in the flow, changes in mass density of the carrier phase due to evaporation and condensation are absent and the agreement between the compressible and the incompressible formulation is expected to be closer than in case of droplets. Although we investigate in this paper situations with relative humidity of 100% for which the mass transfer between the liquid and gaseous phases is quite small, we do observe that the agreement between the two formulations is indeed better for solid particles than for evaporating droplets. In Figure 2.10 we compare the Nusselt number obtained with the two formulations and confirm that the differences in case particles are dispersed are considerably smaller than in case of droplets. As may be inferred, the Nusselt number in the well-developed stages the droplets cases differ in absolute value by about 3-4, while the differences in the particle cases is reduced to well below 1.

The viscous heating term which is present in the compressible formulation and absent in the incompressible transfers kinetic energy into heat. In case when all kinetic energy would be transferred into heat, the gas temperature would change on the order of 0.05%. We also performed a simulation without the viscous heating term in the compressible model. The results of this simulation demonstrate that the viscous heating term is negligible when it comes to assessing the agreement between the two formulations.

2.5.3 Water vapor

In this subsection characteristics of the water vapor distribution will be shown. The temperature gradient in the wall-normal direction causes evaporation of droplets in the region near the hot wall and condensation of vapor on the droplets in the region near the cold wall.

To understand this more precisely we consider the region near the hot wall. The temperature increase in this region causes an increase of the saturation pressure according to Antoine's relation. Consequently, the vapor mass fraction at the surface of the droplet increases as well and this leads to evaporation. The opposite situation, i.e., condensation of water vapor, is

Fig. 2.5: Gas temperature averaged over the homogeneous directions as a function of the wall-normal coordinate at different times. Dashed lines: initial profile obtained without droplets, solid lines: evolution of the profile in time, shown at $t = n\Delta t$ with $\Delta t = 1$ s. The arrows show the direction of increasing time. (a): $Ma = 0.2$, (b): $Ma = 0.05$.

Fig. 2.6: Gas temperature averaged over the homogeneous directions and over time $[2s; 8s]$ as a function of the wall-normal coordinate. Dashed: incompressible, circles: $Ma = 0.2$; dash-dotted: $Ma = 0.1$; solid: $Ma = 0.05$.

obtained in the region near the cold wall. This creates a vapor mass density gradient in the wall-normal direction of the channel, as is illustrated in Figure 2.11. Moreover, both water vapor mass density, Figure 2.11a, and its root-mean square, Figure 2.11b, show that decreasing compressibility through a decrease of Ma leads to increased correspondence with the incompressible results.

Another quantity that characterizes the presence of water vapor in the carrier gas is the rel-

Fig. 2.7: (a): Evolution of RMS of the gas temperature averaged over the homogeneous directions for $Ma = 0.2$. The dashed line shows the initial profile, solid lines show the profiles at later times. (b): RMS of gas temperature averaged over the homogeneous directions and over time [2s;8s] as a function of the wall-normal coordinate. Dashed: incompressible, circles: $Ma = 0.2$; dash-dotted: $Ma = 0.1$; solid: $Ma = 0.05$.

Fig. 2.8: Nusselt number evolution: (a): Dashed: incompressible, circles: $Ma = 0.2$; dash-dotted: $Ma = 0.1$; solid: $Ma = 0.05$. (b): Solid: compressible, dashed: incompressible. Lines without markers: case 3, squares: case 4, circles: case 5.

ative humidity. The higher temperature at the top wall will mean a locally smaller relative humidity at the same vapor concentration according to Antoine's relation (2.22). The same reasoning leads to a somewhat higher relative humidity near the colder bottom wall. The air near the hot wall can hold more vapor than the air near the cold wall. In Figure 2.12 the results

Fig. 2.9: Gas temperature difference between the two walls, averaged over the homogeneous directions as a function of time. Solid: case 3, squares: case 4, circles: case 5.

Fig. 2.10: Nusselt number evolution for case 5. Solid: compressible, dashed: incompressible. Lines without markers: particles case, squares: droplets case.

of the relative humidity are presented. In the major part of the channel the relative humidity is close to 100%. Figure 2.12a shows that, of the cases considered, the compressible formulation agrees closest with the incompressible model at $Ma = 0.05$. In figure 2.12b the results of cases 4 and 5 are compared. Significantly higher and smaller values of the relative humidity at the cold and hot wall, respectively, are observed in case 4 compared to cases 3 and 5. It was verified that the value of the temperature at the cold wall and the mass density of water vapor near this wall are smaller in case 4 than in case 5, which leads to a higher value of relative humidity by approximately 10%. So, while an increase in the system temperature as in case 5 leads to an increase in Nu , as seen in the previous subsection, an increase in the heat flux through the wall as in case 4 mainly affects the relative humidity.

Fig. 2.11: (a): Mean water vapor mass density averaged over time $[2s, 8s]$ as a function of the wall-normal coordinate. (b): RMS of water vapor mass density as a function of the wall-normal coordinate. Dashed: incompressible, circles: $Ma = 0.2$; dash-dotted: $Ma = 0.1$; solid: $Ma = 0.05$.

2.5.4 Properties of droplets

The evolution of the mean droplet diameter d near the walls, normalized by the initial droplet diameter d_0 , is shown in Figure 2.13a. The near wall regions were chosen for the comparison because it was verified that in the middle of the channel the process of phase transition is occurring at a much lower rate. Figure 2.13a once more establishes that droplets evaporate in the region near the hot wall and water vapor condenses on the droplets near the cold wall. Figure 2.13b shows the evolution of the root-mean square of the normalized droplet diameter. For both the mean and RMS of the droplet diameter, the agreement between the compressible and incompressible formulations improves for lower values of the Mach number. This is particularly strong for the RMS values.

Figure 2.14 demonstrates the results for the mean particle diameter for cases 3, 4 and 5,

Fig. 2.12: Relative humidity ϕ as a function of the wall-normal coordinate. (a): Dashed: incompressible, circles: $Ma = 0.2$; dash-dotted: $Ma = 0.1$, solid: $Ma = 0.05$. (b): Dashed: incompressible; solid: compressible where squares denote case 4 and circles refer to case 5.

illustrating the effect of increasing the heat flux through the walls (case 4) and raising the system temperature (case 5). The differences between the two formulations become more pronounced in case 4, Figure 2.14b. The lines corresponding to case 3 and case 5 almost coincide, which proves the independence of the mean droplet diameter near the walls on the mean temperature in the channel. As observed in the previous subsection, an increased heat flux through the walls mainly affects the mass transfer near the walls.

The effect of turbophoresis is presented in Figure 2.15 where the droplet concentration in the region near the cold wall is shown as a function of time. In order to calculate the droplet concentration the domain was divided into 40 equal bins in the wall-normal direction. The concentration is normalized by the uniform initial concentration. We observe that for both formulations droplets tend to migrate to the walls. We observe significant dynamics in the evolution of the droplet concentration near the wall. Relative to this variability, good agreement is observed between the two models at all values of the Mach number considered, cf. Figure 2.15a. A general ‘bandwidth’ of about 5-10% is observed, which corresponds to the level of variations in the root-mean square of the velocity. In fact, as shown in Kuerten (2006) the concentration of droplets near the walls depends on the gradient of the variance of the wall-normal velocity of the carrier phase. The agreement between the two models at all Mach numbers considered is also seen by the close correspondence of the root-mean square of the wall-normal velocity of the carrier gas averaged over time. Figure 2.15b shows that the agreement between the two models in the normalized concentration near the cold wall does not depend on the test case: the results for cases 3, 4 and 5 almost coincide, i.e., the droplet concentration near the wall is independent of the heat properties of the system.

Fig. 2.13: (a): Normalized mean droplet diameter history. The upper lines: region near the cold wall, bottom lines: region near the hot wall. (b): RMS of the normalized droplet diameter near the cold wall. Dashed: incompressible, circles: $Ma = 0.2$; dash-dotted: $Ma = 0.1$; solid: $Ma = 0.05$.

Fig. 2.14: Normalized mean droplet diameter history. Solid: compressible, dashed: incompressible. Lines without markers: case 3, squares: case 4, circles: case 5. (a): Region near the cold wall, (b): region near the hot wall.

2.6 Conclusions

In this paper two approaches were compared to model turbulent droplet-laden channel flow with phase transition. In one approach, the carrier phase was modeled as a compressible Newtonian fluid and these results were compared with the incompressible model adopted by

Fig. 2.15: History of droplet concentration near the cold wall, normalized with the initial value. (a): Dashed: incompressible, circles: $Ma = 0.2$; dash-dotted: $Ma = 0.1$; solid: $Ma = 0.05$. (b): Solid: compressible, dashed: incompressible. Lines without markers: case 3, squares: case 4, circles: case 5.

Russo et al. (2014). We observed a close agreement of the fluid mechanical aspects between the two formulations, e.g., velocity profiles differing less than 1%, at low Mach numbers. Conversely, the thermal properties of the carrier gas and the mass transfer properties of the dispersed droplets were found to display considerably larger systematic differences, also in the limit of low Mach numbers. For instance, the Nusselt number is predicted about 10% higher in the low-Mach compressible formulation, compared to the incompressible findings. Apart from dependence on the Mach number, also the effects of heat flux variations and raising the system temperature we considered. We increased the value of the heat flux to the walls of the channel by a factor of five in one case and set the mean temperature within the channel equal to 323.15 K instead of 293.15 K in another case. As expected, for these two cases we get more pronounced differences between the two formulations. For the case of increased heat flux to the walls a difference in the mean droplet diameter near the walls on the order of 5% was observed, while for the case of a higher mean temperature we see a significant difference in the Nusselt number of about 15%, showing the relevance of the compressible formulation.

It can be concluded that for the chosen ‘mild’ physical situations as far as mass transfer is concerned, with initial relative humidity equal to 100%, the compressible and incompressible formulations show good qualitative agreement. However, for reliable quantitative predictions of heat and mass transfer the compressible formulation is essential. Current research is dedicated to investigating the effect of stronger mass transfer arising from initial conditions with considerably lower initial values of relative humidity. This is expected to further increase the relevance of compressibility effects associated with independent variations in the mass densities of the carrier gas and the vapor, instead of the strict coupling due to the assumption of divergence free velocity. Results of this study in which we apply the current compressible formulation will be published elsewhere.

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Chapter 3

DNS of turbulent droplet-laden heated channel flow with phase transition at different initial relative humidities

Abstract

In this paper a turbulent channel flow of a mixture of dry air and water vapor with water droplets is examined. Direct numerical simulation is used to quantify the importance of variations in the initial relative humidity. We focus on the droplet behavior along with the thermal properties of the system, such as the Nusselt number. During the initial stages of the simulations droplets evaporate more if the initial relative humidity is lower in order to reach the saturation condition. The difference in the Nusselt number between the cases of the lowest initial relative humidity and the saturation initial condition is on the order of 10% and this is connected with the different total heat capacity of the system. At the same time, we confront compressible and incompressible formulations comparing the results for both phases. A lower initial relative humidity leads to a larger difference in the mean gas mass density between the two formulations because of larger heat and mass transfer. Moreover, we find a larger relative difference in the Nusselt number between the two formulations in case of a lower initial relative humidity. These findings motivate the need to adopt the complete compressible flow model.

3.1 Introduction

Turbulent flow fields laden with a large number of small relatively heavy droplets are present in many applications such as pollutant dispersion in the atmosphere and heat transfer in power stations. The dispersed phase not only undergoes momentum exchange with the carrier phase but, in addition, influences thermal properties of the flow. It is important to investigate how droplets affect the turbulent flow and in this paper we concentrate on the additional dynamic effects of coupling phase transitions to the flow. We compare the influence of differences in the initial relative humidity on the heat and mass transfer characteristics.

In the past fifteen years several studies were done in order to investigate droplet-laden turbulent flows. In 1998 Mashayek conducted an Euler-Lagrange simulation study of homogeneous turbulence with two-way coupling in momentum, mass and energy. A study of the mixing layer with embedded evaporating droplets was done by Miller and Bellan (1998). In 2010 Masi et al. investigated the interaction of a non-isothermal droplet-laden turbulent pla-

nar jet with a cloud of inertial evaporating droplets.

In this study we focus on wall-bounded turbulence by considering turbulent channel flow. We incorporate a dispersed droplet phase undergoing phase transition. As a point of reference we consider the flow of water droplets in air, in which the presence of water vapor is accounted for. Throughout the paper the carrier phase or carrier gas denotes a mixture of dry air and water vapor while water droplets will be referred to as the dispersed phase. The top wall of the channel is heated uniformly and the bottom wall is cooled in such a way that the total energy of the system is conserved (Bukhvostova et al. 2014a). This leads to a temperature gradient in the wall-normal direction; in addition droplets tend to evaporate near the upper wall and water vapor tends to condense near the bottom wall. The key difference between the previously mentioned studies and the current is that we consider conditions in which not only evaporation of droplets but also their growth by condensation of the vapor phase is relevant. The presence of phase transitions raises the question whether or not to include explicit compressibility of the carrier phase. The requirement of a constant mass density of the carrier phase in an incompressible formulation implies that the local changes in the mass density of pure air and of water vapor cancel each other precisely throughout the domain. An incompressible model was developed for this problem by Russo et al. (2014). In Bukhvostova et al. (2014a) we confronted the incompressible model with the fully compressible description, analyzing the consequences of non-constant mass density of the carrier gas and discussing for which quantities and under what conditions the full compressible formulation becomes essential. We performed a comparison between the results of the two formulations for “mild” initial conditions in the sense that mass transfer from the liquid to the vapor phase is modest. This was achieved by selecting room temperature, atmospheric pressure and 100% relative humidity (Bukhvostova et al. 2014a). We consider the Nusselt number in order to quantify the heat transfer between the walls of the channel. For these initial conditions we found a difference on the order of 10% in the Nusselt number in the well-developed stages of the flow. We further investigated the agreement between the results from the two models increasing the value of the heat flux through the walls and increasing the mean temperature in the channel. More significant differences were observed: a difference on the order of 15% in the Nusselt number in the case of higher mean temperature and 5% difference in the mean droplet diameter near the walls in case of an increased heat flux.

These differences motivate us to investigate more “severe” physical cases of lower values of initial relative humidity varying it between 100% and 50%. The system tends to reach saturation independently of the initial relative humidity. The amount of water vapor in the carrier gas is increased by the evaporation of droplets and this process is more intense if the initial relative humidity is lower. In this paper we will study thermal properties of the carrier phase and droplet behavior for lower values of the initial relative humidity and also quantify the difference between the results from the two formulations for these cases.

The organization of this paper is as follows. In Section 3.2 the mathematical model is formulated for the coupled droplet-carrier gas system and the numerical methods for both formulations are presented. The initial conditions for the two models are described in Section 3.3. The differences in the behavior of the system under different initial conditions are discussed in Section 3.4. A comparison of the results from the two formulations is presented in Section 3.5. Finally, concluding remarks are collected in Section 3.6.

3.2 The governing equations and numerical methods

The models for the carrier phase are somewhat different in the compressible and incompressible formulations while the dispersed phase is modeled by the same set of ordinary differential equations in both models. The compressible model and the corresponding numerical method are the same as in Bukhvostova et al. (2014a) and the incompressible model is the same as in Russo et al. (2014). For sake of completeness we briefly recapitulate them here.

3.2.1 The carrier phase in the compressible formulation

The carrier phase is a water vapor-air system in a channel, bounded by two parallel horizontal plates. In Figure 3.1 a sketch of the flow domain is presented. The domain has a size of $4\pi H$ in the streamwise direction, which is denoted by x , and $2\pi H$ in the spanwise direction, z , where H is half the channel height. In addition, y is the coordinate in the wall-normal direction. We use periodic boundary conditions in the homogeneous directions (Kim et al. 1987) and no-slip conditions at the walls. A constant heat flux $\dot{Q}$ is applied through the walls. It is equal on both walls in order to conserve the total energy of the system.

The carrier gas is treated in the Eulerian manner as a compressible Newtonian fluid. We impose conservation of mass, momentum, total energy and water vapor. The equations can be written as (Miller and Bellan 1998):

$$\partial_t \rho + \partial_j(\rho u_j) = Q_m \quad (3.1)$$

$$\partial_t(\rho u_i) + \partial_j(\rho u_i u_j) = -\partial_j \pi_{ij} + F_i + Q_{mom,i} \quad (3.2)$$

$$\partial_t e_t + \partial_j(\rho u_j e_t) = -\partial_j q_j - \partial_j(u_i \pi_{ij}) + Q_e \quad (3.3)$$

$$\partial_t(\rho Y_v) + \partial_j(\rho u_j Y_v) = -\partial_j J_{v,j} + Q_m \quad (3.4)$$

where $Q_m, Q_{mom,i}, Q_e$ are sink/source terms expressing the two-way coupling between the phases. These will be described later. In addition, (ρ, u_j, e_t, Y_v) are the carrier phase mass density, components of the velocity, total energy density and vapor mass fraction, respectively. Moreover, π_{ij} defines pressure and viscous contributions to the momentum flux; we use Sutherland's law to compute the dynamic viscosity. The term F_i is an external force density which is obtained from the conservation of total streamwise momentum. In addition, q_j denotes the components of the heat flux vector, which consists of heat transport by conduction and by diffusion and the vector J_v defines the diffusive mass flux of water vapor. The pressure and temperature of the carrier phase are denoted by p and T . The vapor mass fraction, p and T are connected by the ideal gas law for an air-water vapor mixture.

We incorporate the temperature dependence of thermophysical properties such as the thermal conductivity K , diffusivity D and dynamic viscosity μ . In fact, we adopt the Sutherland law for the dynamic viscosity μ (Sutherland 1893) and keep the ratio of K and this dynamic viscosity constant. Similarly, the thermal diffusivity D is allowed to depend on temperature such that the ratio $\rho D/\mu$ is constant. Simulations reported in this paper are done under quite small temperature differences of up to approximately 3K. It was found in Bukhvostova et al. (2014a) that compared to a simulation in which the thermophysical properties are kept constant differences are less than 0.001% for several mean values. At larger temperature differ-

ences between the walls of up to 40K, as studied, e.g., by Zonta and Soldati (2014), inclusion of the temperature dependency of K , D and μ was found to be more important, leading to changes of up to 30% in heat and momentum transfer coefficients arising from variations in local thermophysical properties on the order of 50%.

The system of governing equations (3.1)-(3.4) is made non-dimensional using a set of reference scales of the system as will be further specified in Section 3.3. As a result, the final system of equations contains the Prandtl number Pr , the Mach number Ma , the Schmidt number Sc and the Reynolds number Re .

Fig. 3.1: The computational domain

3.2.2 The carrier gas in the incompressible formulation

In the model by Russo et al. (2014) the carrier gas is also considered in the Eulerian way. The continuity equation and the Navier-Stokes equation in the rotational form are used along with the temperature equation and vapor mass density equation for $(\rho, \mathbf{u}, T, \rho Y_v)$:

$$\nabla \cdot \mathbf{u} = 0 \quad (3.5)$$

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + \boldsymbol{\omega} \times \mathbf{u} + \nabla P \right) = \mu \Delta \mathbf{u} + \rho \mathbf{F} + \mathcal{L}_{\mathbf{u}} \quad (3.6)$$

$$\hat{c}_v \left(\frac{\partial T}{\partial t} + \nabla \cdot (\mathbf{u} T) \right) = k \nabla^2 T + \mathcal{L}_{\text{wd}} + \mathcal{L}_{\text{diff}} + \mathcal{L}_{2\text{way}} \quad (3.7)$$

The equation for the vapor mass density is the same as in the compressible formulation. In (3.6) $\boldsymbol{\omega}$ stands for the vector of vorticity $\boldsymbol{\omega} = \nabla \times \mathbf{u}$, $P = p_{st} + \frac{1}{2} \rho \mathbf{u}^2$, μ is the dynamic

viscosity of the gas, p_{st} is the static pressure while $\frac{1}{2}\rho\mathbf{u}^2$ is the dynamic pressure and $\mathbf{F}$ denotes the driving force obtained from the condition of constant carrier gas flow rate. The term $\mathcal{L}_{\mathbf{u}}$ expresses the momentum exchange between the two phases. Moreover, $\hat{c}_v$ stands for the heat capacity at constant volume of the air-water vapor mixture:

$$\hat{c}_v = \rho(1 - Y_v)c_{v,a} + \rho Y_v c_{v,v} \quad (3.8)$$

where $c_{v,a}$ and $c_{v,v}$ are the specific heat of air and water vapor, respectively.

The term $\mathcal{L}_{\text{wd}}$ represents the transport of energy due to diffusion of water vapor and includes the dependence of the gas thermal conductivity k on the vapor mass density (Russo et al. 2014). In addition, the term $\mathcal{L}_{\text{diff}}$ denotes the contribution to the temperature change from diffusion of vapor and $\mathcal{L}_{\text{2way}}$ is the contribution from the energy exchange between the two phases.

3.2.3 The dispersed phase

The dispersed phase of the system consists of water droplets which are assumed to be spherical and are treated with a point-particle approach. In the current study the droplet volume fraction is chosen to fluctuate around 10^{-4} and therefore we consider two-way coupling according to the classification proposed by Elghobashi (1994).

In the Lagrangian method for the droplets adopted here a system of ordinary differential equations for each droplet is obtained following the model used in Miller and Bellan (1998) and Masi et al. (2010). The location of a droplet is governed by the kinematic condition:

$$\frac{d\mathbf{x}_i(t)}{dt} = \mathbf{v}_i \quad (3.9)$$

where $\mathbf{x}_i$ is the location and $\mathbf{v}_i$ is the velocity of droplet i . Maxey and Riley (1983) derived the equation of motion for a sphere in a non-uniform flow. In the water-air system droplets have a much higher mass density than the carrier fluid and, consequently, the Stokes force acting on a droplet is dominant (Armenio and Fiorotto 2001). We solve the following equation of motion with the standard Schiller-Naumann drag correction (Schiller and Naumann 1933):

$$\frac{d\mathbf{v}_i}{dt} = \frac{\mathbf{u}(\mathbf{x}_i, t) - \mathbf{v}_i}{\tau_{d,i}} (1 + 0.15\text{Re}_{d,i}^{0.687}) \quad (3.10)$$

where $\mathbf{u}(\mathbf{x}_i, t)$ is the velocity of the carrier gas at the droplet position. Moreover, $\tau_{d,i} = \rho_l d_i^2 / (18\mu)$ defines the droplet relaxation time where ρ_l and d_i stand for liquid water mass density and droplet diameter of droplet i , respectively. In addition, $\text{Re}_{d,i}$ is the droplet Reynolds number based on the diameter of the droplet and on the relative velocity of droplet with respect to the local instantaneous flow:

$$\text{Re}_{d,i} = \frac{d_i \rho |\mathbf{u}(\mathbf{x}_i, t) - \mathbf{v}|}{\mu} \quad (3.11)$$

Next to the change of droplet velocity and position we also take into account how its energy, given by $E_i = c_l m_i T_i$, changes in time. Here, c_l is the specific heat of liquid water and m_i , T_i are droplet mass and temperature, respectively. We incorporate both mechanisms for energy changes: mass transfer by phase change and heat exchange by convection at the droplet surface:

$$\frac{d}{dt} E_i = h_v \frac{dm_i}{dt} + h_m A_i (T(\mathbf{x}_i, t) - T_i) \quad (3.12)$$

where $h_v = \lambda_0 + c_{pv} T_i$ denotes the specific enthalpy of water vapor. In the current study we use the following correlation for the heat transfer coefficient h_m for forced convection around a sphere (Bird et al. 1960, page 439):

$$\frac{h_m d_i}{K} = 2 + 0.60 \text{Re}_{d,i}^{1/2} \text{Pr}^{1/3} \quad (3.13)$$

Finally, A_i denotes the surface area of droplet i and $T(\mathbf{x}_i, t)$ the carrier phase temperature at the droplet position.

In order to complete the system of equations we still require an expression for dm_i/dt , the rate of evaporation and condensation of a droplet. We use the following equation (Bird et al. 1960, page 711):

$$\frac{dm_i}{dt} = -\frac{m_i \text{Sh}_{d,i}}{3 \tau_{d,i} \text{Sc}} \ln \left(\frac{1 - Y_{v,\delta,i}}{1 - Y_{v,s,i}} \right) \quad (3.14)$$

where $Y_{v,\delta}$ and $Y_{v,s}$ are the vapor mass fractions at a distance δ from the surface of the droplet and on the surface of the droplet, respectively. The vapor boundary layer thickness around a droplet is denoted by δ . For the Sherwood number of a droplet we use the correlation for a sphere (Bird et al. 1960):

$$\text{Sh}_{d,i} = 2 + 0.60 \text{Re}_d^{1/2} \text{Sc}^{1/3} \quad (3.15)$$

The vapor mass fraction at the surface $Y_{v,s}$ corresponds to thermodynamic equilibrium at the surface, which determines the saturation vapor pressure. $Y_{v,s}$ is found using the saturation pressure $p_{v,sat}$ following from Antoine's relation (Antoine 1888):

$$p_{v,sat} = 10^5 \exp \left(A - \frac{B}{C + T_i} \right) \quad \text{in Pa} \quad (3.16)$$

where $A = 11.6834$, $B = 4089.59 \text{ K}$, $C = 500.02 \text{ K}$ and T_i is taken in Kelvin, in combination with the ideal gas law for water vapor while $Y_{v,\delta}$ is considered as the vapor mass fraction of the carrier phase at the position of the droplet.

Finally, the governing equations in both formulations contain two-way coupling terms which are found from the conservation of mass, momentum and internal energy of the system. The mathematical expressions for them contain delta-functions in both models which reflect that the two-way coupling terms act on the carrier phase only at the locations of the droplets (Bukhovostova et al. 2014a). For example, the two-way coupling term in continuity equation (3.1) and in total energy density equation (3.3) are given by expression:

$$Q_m = - \sum_i \frac{dm_i}{dt} \delta(\mathbf{x} - \mathbf{x}_i) \quad (3.17)$$

$$Q_e = - \sum_i \frac{d}{dt} (c_l m_i T_i) \delta(\mathbf{x} - \mathbf{x}_i) \quad (3.18)$$

where the sum is taken over all droplets in the domain. The expressions for the two-way coupling terms in the incompressible formulation are derived in the same way.

3.2.4 Numerical methods

The incompressible and compressible models are simulated using different numerical methods. The incompressible formulation adopts a pseudo-spectral method for the carrier phase as described in Russo et al. (2014) and Kuerten (2006). In the two periodic directions a Fourier-Galerkin approach is used, while a Chebyshev-collocation approach is applied in the wall-normal direction. The droplet equations are integrated in time with the same three-stage Runge-Kutta method as used for the convective terms in the carrier phase equations. The viscous terms and pressure are integrated in time with the implicit Crank-Nicolson method. The pressure is found at each time level from the divergence-free condition for the velocity, following the approach proposed by Kleiser and Schumann (1980).

The numerical model for the compressible carrier phase adopts explicit four-stage low-storage Runge-Kutta time-stepping with weights equal to 1/4, 1/3, 1/2 and 1 and a second order finite volume discretization (Vreman et al. (1992)). A uniform grid is used in the two periodic directions while in the wall-normal direction a non-uniform grid is applied which is finer near the walls. The variables are stored in the centers of the cells. For each of the cells we integrate the governing equations (3.1)-(3.4) for the carrier phase in the conservative form over the volume of the cell. In both models we use 128 grid points in each direction.

The system of ordinary differential equations for the droplets is integrated in time applying the same four-stage compact Runge-Kutta method as used for the gas equations. The right-hand sides of the droplet equations contain gas properties at droplet location. In order to determine these, tri-linear interpolation is applied in both formulations (Marchioli et al. 2008).

3.3 Initial conditions of the simulations

In this section the initial conditions for the simulations will be described and motivated, both for the compressible and the incompressible formulation.

The initial condition for the simulations with the two models is a snapshot of the solution in the statistically steady state of the corresponding system of equations in the absence of droplets and with adiabatic boundary conditions, as obtained with the respective compressible and incompressible model. For the incompressible model this solution has a constant mass density and temperature. The solution in the steady state of the system (3.1)-(3.3) has a non-constant gas mass density and temperature. The difference is caused by a slight variation of

mass density due to compressibility which is characterized by the Mach number.

The simulations are performed at a fixed bulk Reynolds number $Re_b = 2333$ the same as in Marchioli et al. (2008). The Reynolds number defines the reference velocity u_{ref} which is taken as the initial bulk velocity of the carrier gas:

$$u_b = \frac{Re_b \mu(T_{ref})}{L \rho_{ref}} \quad (3.19)$$

where the reference temperature T_{ref} is chosen to be equal to 293.15 K and the dynamic viscosity at the reference temperature $\mu(T_{ref})$ is found by applying Sutherland's law (Sutherland 1893). The reference length L is chosen as half the channel height H ; specifically, we consider a water-air system flowing between a channel with $H = 2$ cm. The reference mass density ρ_{ref} is the initial mass density of the mixture.

In this study we quantify the effect of changes in the initial relative humidity. The relative humidity ϕ characterizes the amount of water vapor in the channel. It is defined as the ratio of the partial vapor pressure p_v in the air-water vapor mixture to the saturated vapor pressure $p_{v,sat}$ at the prescribed temperature, $\phi = p_v / p_{v,sat}$. We first find the saturation pressure at the reference temperature $p_{v,sat}(T_{ref})$ using Antoine's relation (3.16). Consequently, we know the partial pressure of water vapor which is equal to $\phi p_{v,sat}(T_{ref})$. From the equation of state for water vapor we may find the initial vapor mass density $\rho_v(T_{ref})$ in the channel corresponding to the chosen relative humidity:

$$\rho_v(T_{ref}) = \rho Y_v(T_{ref}) = \frac{\phi p_{v,sat}(T_{ref})}{R_{water} T_{ref}} \quad (3.20)$$

where R_{water} denotes the specific gas constant of water. We vary the initial ϕ in this study, choosing values of 100%, 75% and 50%. These cases will be called RH100, RH75 and RH50, respectively. In Table 3.1 the initial vapor mass density $\rho_v(T_{ref})$ at the reference temperature is shown.

In (3.19) the reference density ρ_{ref} is chosen as the initial mass density of the mixture. The initial pressure of the air-water vapor mixture in the channel p is equal to atmospheric pressure. We use Dalton's law for the mixture and the equation of state for dry air and vapor to substitute the partial pressure of the mixture components:

$$p = R_{air} \rho_{air} T_{ref} + R_{water} \rho_v(T_{ref}) T_{ref} \quad (3.21)$$

where R_{air} stands for the specific gas constant of dry air. In addition, ρ_{air} and ρ_v define the mass density of dry air and water vapor, respectively. We express the mass density of pure air from (3.21):

$$\rho_{air} = \frac{p - R_{water} \rho_v(T_{ref}) T_{ref}}{R_{air} T_{ref}} \quad (3.22)$$

Knowing $\rho_v(T_{ref})$ from (3.20), we can find the initial mass density of dry air and, consequently, the initial mass density of the mixture:

$$\rho = \rho_{air} + \rho_v(T_{ref}) \quad (3.23)$$

Table 3.1 shows the reference mass density. Because of the different initial amount of water vapor in the mixture, $\rho_v(T_{ref})$, the reference mass density is different in each case. Consequently, it leads to different initial bulk velocities as it is seen from (3.19).

The Mach number depends on the Reynolds number and it is calculated according to:

$$\text{Ma} = \frac{u_{ref}}{c(T_{ref})} = \frac{\text{Re}_b \mu(T_{ref})}{L \rho_{ref} c(T_{ref})} \quad (3.24)$$

where $c(T_{ref})$ is the speed of sound at the reference temperature which is computed using the following:

$$c(T_{ref}) = \sqrt{\frac{\gamma_{air} R_{air} T_{ref}}{M_{air}}} \quad (3.25)$$

where γ_{air} is defined as the ratio between the specific heats at constant pressure and constant volume of air and M_{air} is the molar mass of air. The Mach number calculated using (3.24) is approximately equal to 0.005. Because of the stability condition of the explicit time-integration method of the compressible formulation this value of the Mach number is too low to allow full simulations within a reasonable amount of time. Instead, we choose $\text{Ma} = 0.05$. In (Bukhvostova et al. 2014a) it was shown that at this Mach number all gas and droplets characteristics that would arise at $\text{Ma} = 0.005$ are accurately approximated.

The other non-dimensional parameters of the simulations are shown in Table 3.1. The Prandtl number is defined in the following way:

$$\text{Pr} = \frac{c_{pa} \mu(T_{ref})}{K(T_{ref})} \quad (3.26)$$

where c_{pa} is the specific heat of air at constant pressure and K is the thermal conductivity of the carrier gas. In order to compute this we use the formula for the thermal conductivity of a mixture (Bird et al. 1960, page 276) which contains the mass density of vapor and the carrier gas. Since these values are different for different initial relative humidity, we get different values of the Prandtl number for the three cases. The Schmidt number is defined as:

$$\text{Sc} = \frac{\mu(T_{ref})}{\rho_{ref} D(T_{ref})} \quad (3.27)$$

where D stands for the diffusion coefficient of water vapor in air and it is calculated using Chapman-Enskog theory for gases (Cussler 1997). The presence of ρ_{ref} in (3.27) leads to different values of the Schmidt number in the three cases considered.

We randomly distribute $N_{\text{drop}} = 2,000,000$ identical droplets over the volume of the channel. For both models the initial droplet diameter is given by $d_i/H = 3.09 \times 10^{-3}$. The corresponding initial volume fraction of droplets is equal to 1.9×10^{-4} and the mean volume fraction fluctuates around this value during the simulations. According to the classification proposed by Elghobashi (1994) this volume fraction corresponds to the regime when two-way coupling is required and the effects of collisions between droplets are negligible. The usage of the point-particle approach is justified by the ratio of the droplet diameter and the minimum Kolmogorov length scale along the wall-normal direction. This ratio is equal to 0.3 and shows that the point-particle approach is valid (Marchioli et al. 2008), (Elghobashi 1994). Velocity

and temperature of the droplets are initialized using the carrier gas values at the droplet locations.

case	RH100	RH75	RH50
T_{ref} (K)	293.15	293.15	293.15
$\rho_v(T_{ref})$ (kg/m ³)	0.0169	0.0127	0.0085
ρ_{ref} (kg/m ³)	1.194	1.8998	1.1855
u_b (m/s)	1.8246	1.8311	1.8377
Re_b	2333	2333	2333
Ma	0.05	0.05	0.05
Pr	0.7425	0.7395	0.7365
Sc	0.62883	0.63055	0.6328

Table 3.1: Parameters of the test cases

3.4 Heat and mass transfer at different initial relative humidities

In this section we describe the difference in the behavior of the droplets and the carrier gas in cases RH50, RH75 and RH100. Throughout this and the next section we show averaged quantities of the carrier and dispersed phases. The carrier gas quantities are averaged over the homogeneous directions. For the dispersed phase we use 40 equal-sized slabs in the wall-normal direction and average over all the droplets contained in a certain slab at a certain time. The averages in both phases are denoted by $\langle \cdot \rangle$.

In all cases the heat flux applied to the walls causes a temperature gradient in the channel: we get a higher temperature near the top wall which will be called the hot wall and lower near the bottom wall referred to as the cold wall. This temperature profile leads to the development of a vapor mass density gradient across the channel; droplets tend to evaporate near the hot wall and water vapor tends to condense near the cold wall.

In case RH50 droplets evaporate more than in case RH100, Figure 3.2. The figure confirms what is predicted by (3.14). The driving force in (3.14) is the difference $Y_{v,\delta} - Y_{v,s}$. For an unsaturated initial condition $Y_{v,\delta}$ is smaller than $Y_{v,s}$ and this leads to negative values of $\frac{dm_i}{dt}$. The smaller initial relative humidity leads to a smaller value of $Y_{v,s}$ and, consequently, to a more negative $\frac{dm_i}{dt}$. A clear difference in the droplet mean diameter is seen in the transient phase of the simulations, which lasts about 0.1 s. Near both walls droplets shrink for case RH50, which is caused by the initial low value of the relative humidity. The system tends to approach a saturation condition, which is independent of the initial relative humidity level. This is achieved by droplet evaporation which continues until the final relative humidity reaches approximately 100%. The change in the droplet mean diameter near the cold wall until time 0.1 s in case RH50 is twice larger than in case RH75. Consequently, the further the initial system is from saturation, the more intense the evaporation of droplets during the initial times of the simulations is. Later in time the system remains close to saturation and droplets start to grow in the region near the cold wall.

The behavior of the relative humidity as a function of time is connected to the behavior of the

droplets, Figure 3.3. The behavior of the relative humidity can also be predicted analytically to a good approximation. For that we may reason as follows. Combining equations (3.1) and (3.4), we obtain the equation for the vapor mass fraction change:

$$\partial_t Y_v + u_j \partial_j Y_v = -\frac{\partial_j J_{v,j}}{\rho} + \frac{Q_m(1 - Y_v)}{\rho} \quad (3.28)$$

The convective and diffusive terms in (3.28) can be neglected since the initial conditions lead to a small gradient of the vapor mass fraction so that the source term in (3.28) is dominant. The typical values of Y_v are small compared to 1, Table 3.1. Consequently, the behavior of Y_v is well approximated by:

$$\frac{dY_v}{dt} = \frac{Q_m}{\rho} \quad (3.29)$$

Substituting two-way coupling term and using a Taylor expansion for $\ln\left(\frac{1-Y_{v,\delta}}{1-Y_{v,s}}\right)$ in equation (3.14) we obtain:

$$\frac{dY_v}{dt} = \frac{Y_{v,s} - Y_{v,\delta}}{\tau} \quad (3.30)$$

where τ stands for the evaporation relaxation time which is equal to:

$$\tau = \frac{3\tau_{d,i}\rho Sc}{m_i Sh_{d,i}} \frac{V}{N_{\text{drop}}} \quad (3.31)$$

We divide equation (3.30) by the saturation vapor mass fraction $Y_{v,s}$ and obtain an equation for the change of the relative humidity:

$$\frac{d\phi}{dt} = \frac{1 - \phi}{\tau} \quad (3.32)$$

For our initial conditions we obtain $\tau = 0.0658$ s. The insert in Figure 3.3a shows the analytical solution of (3.32) and the numerical results in the middle of the channel: a very close agreement is observed.

One observes a close agreement in the relative humidity near the walls between cases RH50 and RH100 at later times of the simulations. However, there is a significant difference in the droplet diameter history near the walls. These quantities are connected through the water vapor. In all cases the system tends to approach the saturation condition. In cases with lower initial relative humidity droplets evaporate initially much more than in case RH100. Further in time, the approximate saturation condition, reached at 0.1 s, is maintained: the water vapor which was obtained by droplet evaporation in cases RH50 and RH75 satisfies the saturation condition and consequently, there is less water in the form of droplets.

Fig. 3.2: Normalized droplet diameter history near the walls. Dashed: RH100, solid: RH50. Squares: hot wall, without squares: cold wall. Circles: simulations of RH50 on $192 \times 192 \times 192$ grid with compressible solver.

Fig. 3.3: Relative humidity history near the walls. Square marked lines: RH100, lines without markers: RH50. (a): region near the cold wall, (b): region near the hot wall. (a) insert: relative humidity history in the middle of the channel, dashed: analytical solution, circles: numerical result.

3.5 Comparison of heat and mass transfer obtained with compressible and incompressible formulations

In this section we will quantify the effects of compressibility of the carrier gas on the mean gas temperature, Nusselt number and droplet size probability density function by comparing

the agreement between the results of the compressible and incompressible formulations for all three cases.

3.5.1 *The need for a fully compressible formulation*

There are three main differences between compressible and incompressible flows: a constant mass density, a zero divergence of the velocity and an infinite speed of sound in incompressible flow. The incompressible formulation for the carrier phase adopted by Russo et al. (2014) implies that all instantaneous changes in the local mass density of air and water vapor cancel each other precisely throughout the domain. This is required to maintain a constant mass density of the carrier phase. In our problem the carrier gas mass density is not strictly constant. We compared the mean gas mass density as a function of the wall-normal coordinate for all cases. The results from the previous section show that during the same time there is a larger change in the amount of water vapor in the system in case RH50 than in case RH100. Since water vapor contributes to the total mass density of the carrier phase, which is considered constant in the incompressible formulation, one expects bigger differences in the carrier gas mass density between the compressible and incompressible formulations in case RH50 than in case RH100. The mean mass density of the carrier gas in the well-developed state is shown in Figure 3.4 for cases RH100 and RH50. The maximum relative difference is two times larger in case RH50 than in case RH100 and 1.5 times larger in case RH75 than in case RH100.

In our problem the divergence of the velocity field is not equal to zero because of phase transitions. We compared the RMS of two terms in the continuity equation: $\rho \nabla \cdot \mathbf{u}$ and $\mathbf{u} \cdot \nabla \rho$ as functions of the wall-normal coordinate for cases RH100 and RH50 during the initial stage of the simulations, Figure 3.5. The figure shows that the RMS of the term $\rho \nabla \cdot \mathbf{u}$ in case RH50 is on average ten times larger than other RMS's shown in Figure 3.5. This proves that in case of RH50, where phase transitions are more important the effect of explicit compressibility becomes more pronounced.

Another important difference between the two formulations follows from continuity equation (3.1). For the turbulent channel flow treated with the incompressible formulation the wall-normal component of the momentum of the carrier gas averaged over the periodic directions is always equal to zero as follows from equation (3.5). In the compressible formulation this is approximated only in the statistically steady state. We studied the wall-normal component of the carrier gas momentum averaged over the homogeneous directions and over different time intervals as a function of the wall-normal coordinate in the compressible formulation for case RH100 and RH50, Figure 3.6. The figure shows how the wall-normal momentum component develops in time starting from the initial stage of the simulation until the statistically steady state has been reached. During the initial stage the development of the temperature gradient in the wall-normal direction leads to a mean motion of gas from the hot to the cold wall, since the wall-normal momentum is mostly negative within the channel, Figure 3.6. In the statistically steady state the mean wall-normal momentum profile is close to zero. The amplitude of the mean momentum is larger in case RH50 than in case RH100 during the initial stages of the simulations because of the more intense evaporation and, consequently, larger contribution from the two-way coupling term Q_m in equation (3.1).

The analysis of the divergence of the velocity field and of the wall-normal momentum shows

a clear difference between these terms in the two formulations in case RH100. In case RH50 the difference becomes more pronounced and motivates the usage of the compressible formulation for better quantitative prediction of the system behavior.

Fig. 3.4: Mean gas mass density as a function of the wall-normal coordinate at $t = 2\text{s}$. Dashed: incompressible, solid: compressible. (a): RH100, (b): RH50. Squares: simulation on 192×192 grid with compressible solver.

Fig. 3.5: Solid: RMS of $\rho \nabla \cdot \mathbf{u}$, dashed: RMS of $\mathbf{u} \cdot \nabla \rho$ as a function of the wall-normal coordinate. Circles: RH100, lines without markers: RH50.

Fig. 3.6: Wall-normal momentum of air averaged over the homogeneous directions and over time intervals; solid: [0s;0.1s], circles: [0.2s;0.3s], squares: [0.3s;0.4s], dashed: [1s;1.1s]. (a):RH100, (b): RH50.

3.5.2 Comparison with incompressible model

We compared the compressible and incompressible models in terms of the mean gas temperature at a characteristic time in the statistically steady state of the gas for the three cases considered, Figure 3.7. We quantify the difference between the results of the two formulations by normalizing it with the mean gas temperature difference between the two walls. The maximum relative difference between the two models is approximately equal to 6% in case RH50, 3% in case RH75 and around 2% in case RH100. One can observe a higher mean gas temperature in the channel in the compressible model than in the incompressible in case RH50, figure 3.7c. The equation for the carrier gas temperature change is equation (3.7) and the expressions for the two-way coupling terms in it can be found in Russo et al. (2014). The carrier gas temperature mainly changes because of the two-way coupling term in which the main contribution is $h_m A_i (T(\mathbf{x}_i, t) - T_i)$. We verified with the compressible solver in case RH100 that this term has on average a twice larger absolute value than the term $h_v \frac{dm_i}{dt}$ in equation (3.14). The exchanged energy between the two phases $h_m A_i (T(\mathbf{x}_i, t) - T_i)$ causes a change in energy of the carrier gas quantified by $\hat{c}_p V \rho \frac{dT}{dt}$, where $\hat{c}_p$ denotes the specific heat at constant pressure of the air-water vapor mixture. For the same energy exchange between the two phases we get a smaller change in the gas temperature in case RH50 for the compressible formulation than in the incompressible formulation since the mass density in the compressible formulation is larger than in the incompressible formulation, Figure 3.4b. The difference in the mean temperature becomes more pronounced for RH50, since the difference in gas mass density is largest among the cases considered.

To express the efficiency of the heat transfer between the channel walls we consider the Nusselt number defined in the following way:

$$\text{Nu} = \left(\frac{d\langle T \rangle}{dy} \Big|_{\text{wall}} \right) / \frac{\Delta\langle T \rangle}{2H} \quad (3.33)$$

where $\Delta \langle T \rangle$ is the difference in mean gas temperature between the two walls and the derivative with respect to the wall-normal coordinate in the numerator is averaged over both walls. Figure 3.8 shows how the Nusselt number depends on time for cases RH50 and RH100 in both formulations. The relative difference between the results from the two formulations in the Nusselt number averaged over time interval [2s;5s] is 1.5 times larger in RH50 than in RH100, Table 3.2.

Kuerten et al. (2011) showed that in incompressible flow with solid particles three contributions to the Nusselt number can be distinguished:

$$\text{Nu} = \text{Nu}_{\text{lam}} + \text{Nu}_{\text{turb}} + \text{Nu}_{\text{part}}, \quad (3.34)$$

which denote the Nusselt number for laminar flow, a contribution from turbulence and a contribution from particles. In case of turbulent flow with droplets there are some additional contributions caused by water vapor diffusion and phase change, but these are negligible (Russo et al. 2014). We calculated all three contributions in (3.34) in cases RH100, RH75 and RH50 in the incompressible formulation, Table 3.3, averaging over time interval [2s;5s]. The difference in the resulting Nusselt number between cases RH100 and RH50 is caused by a relative difference on the order of 10% in Nu_{part} while the other contributions are virtually unchanged. In Kuerten et al. (2011) a simplified expression for Nu_{part} is given:

$$\text{Nu}_{\text{part}} = - \int_{-H}^H \int_{-H}^y \frac{2\pi \langle n(s) d_i (T(\mathbf{x}_i, t) - T_i) \rangle_t}{\langle \Delta T \rangle_t} ds dy, \quad (3.35)$$

where $n(s)$ denotes the droplet concentration as a function of the wall-normal coordinate and $\langle \cdot \rangle_t$ stands for averaging over time and the homogeneous directions. We investigated various factors in the integrand of (3.35): average droplet concentration, droplet diameter and the relative temperature normalized by the averaged temperature difference between the walls as functions of the wall-normal coordinate. In order to compute the droplet concentration we used slabs in the wall-normal direction which are defined by the Chebyshev collocation points. In this way we have more slabs near the channel walls and the effect of turbophoresis can be accurately taken into account (Kuerten 2006). The concentration is normalized by the uniform initial concentration. For the computation of the relative temperature which is defined as $\frac{T(\mathbf{x}_i, t) - T_i}{\Delta T}$, we also used the slabs which are defined by the Chebyshev collocation points in order to have the averaged droplets and gas quantities at the same locations.

While the droplet concentration and diameter show close agreement in cases RH50 and RH100, Figure 3.9a and 3.9b, the normalized relative temperature is quite different, especially in the regions near the walls, Figure 3.9c.

The rate of mass transfer near the walls is higher in case RH100 than in case RH50 and this is explained by the following reasoning. After the initial evaporation phase of case RH50 the two cases have a different mean gas temperature of approximately 5K. In Russo et al. (2014) it is explained that a higher mean temperature leads to a larger mass transfer near the walls, and hence to a larger temperature difference between droplets and gas. This is caused by the nonlinearity of Antoine's law. The consequence of this is that the lower mean temperature level of case RH50 leads to a smaller Nusselt number than in case RH100. We also performed a simulation with a smaller reference temperature equal to the mean temperature in the steady state in the RH50 case, but with an initial relative humidity of 100%. In the steady state the Nusselt number in this simulation is close to the Nusselt number in case RH50.

We also considered the droplet size probability density function (PDF) near the hot wall at

different times, Figure 3.10. In order to compute this PDF, the wall-normal direction was divided into 64 equidistant slabs and for each slab the number of droplets within a certain diameter range was computed. This range is calculated based on the maximum and minimum droplet diameter in each slab and the whole diameter range of each slab is divided into 100 equal bins. The size is normalized with the initial droplet diameter, d_0 . We compare the droplet size PDF from the two formulations in case RH50 and RH100 at 0.1 s and at 2 s. At both times and for both initial relative humidities we observe close agreement between the results. Figure 3.10 illustrates in a more detailed way Figure 3.2. Droplets evaporate more in RH50 than in RH100 at 0.1 s as Figure 3.10a shows. In addition, the transfer of liquid water from the droplets to the vapor phase is maintained in time: the PDF's for RH50 are shifted over approximately the same distance relative to the PDF's for RH100 at the two moments in time.

	RH50	RH100
compr	13.91	15.53
incompr	13.04	14.83

Table 3.2: Nusselt number averaged over [2 s;5 s] in the two formulations in cases RH50 and RH100.

case	Nu	Nu _{lam}	Nu _{turb}	Nu _{part}
RH100	14.5	1.0	2.5	11.0
RH75	14.2	1.0	2.6	10.6
RH50	13.4	1.0	2.6	9.8

Table 3.3: Contributions in the Nusselt number for cases RH100, RH75 and RH50. Time averaging is performed for the time interval [2s;5s].

3.5.3 Simulation on a finer grid

The differences between the results from the two formulations which will be discussed in the next subsection are not caused by the different numerical approaches but by the physics of the occurring events. We verified it performing the simulations also on a finer grid with 192 points in each direction with the compressible solver for case RH50. Figures 3.2, 3.4b and 3.11 show very close agreement between the results from the two grids in the compressible solver. Consequently, the comparison of the results from the two formulations is not influenced by the difference in the applied numerical methods but mainly reflects the physical differences.

Fig. 3.7: Mean gas temperature as a function of a wall-normal coordinate. Dashed: incompressible, solid: compressible. (a): RH100, (b): RH75, (c): RH50.

3.6 Concluding remarks

In this paper we investigated the behavior of turbulent droplet-laden channel flow undergoing phase transitions at different initial relative humidities and confronted incompressible and compressible formulations to model the system. We performed the simulations with initial values of relative humidity equal to 100%, 75% and 50% which are denoted as cases RH100, RH75 and RH50.

We observe qualitative differences during the initial stages of the simulations when in cases RH50 and RH75 droplets evaporate more before the system reaches saturation. Consequently, it leads to a larger amount of water vapor in the carrier phase which leads to larger variations of the carrier gas mass density. More significant differences between the results of the two models were found in thermal quantities such as mean gas temperature and the Nusselt num-

Fig. 3.8: Nusselt number history. Dashed: incompressible, solid: compressible formulation. Square marked lines: RH100, lines without markers: RH50.

ber for cases RH50 and RH75 than for case RH100. The relative difference in the Nusselt number averaged over time in its steady state is 1.5 times larger in case RH50 than in RH100. Consequently, the differences between the results from the two formulations for cases RH75 and RH50 in the respect to the differences in case RH100 may need the compressible formulation for better quantitative prediction.

Fig. 3.9: (a) Droplet concentration normalized by the initial number of droplets in a slab, (b) droplet diameter, (c) normalized relative temperature, averaged in time and homogeneous directions as functions of the wall-normal coordinate. Solid line: RH100, dashed line: RH50.

Fig. 3.10: Droplet size PDF near the hot wall. (a): at 0.1 s, (b): at 2 s. Solid: compressible formulation, dashed: incompressible.

Fig. 3.11: Droplet size PDF near the hot wall at 0.1s for RH50. Solid: simulations on $128 \times 128 \times 128$ grid, dashed: simulations on $192 \times 192 \times 192$ grid; both with compressible solver.

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Chapter 4

Low Mach number algorithm for droplet-laden turbulent channel flow including phase transition

Abstract

In this study we propose a new numerical algorithm for droplet-laden turbulent channel flow with phase transitions at low Mach numbers. The carrier gas is treated as compressible flow. In order to avoid very small time steps at low Mach numbers that would arise from stability requirements associated with explicit time-stepping we propose a new semi-explicit time integration method, applied to the low Mach number compressible flow equations. We perform a perturbation analysis in powers of the Mach number of the system of governing equations. The obtained decomposition of pressure into a space-independent part and a hydrodynamic part permits to apply a special pressure-based time integration algorithm for compressible flows at low Mach numbers. An important feature of the new numerical approach is the independence of the maximum allowed time step on the Mach number. In this study we validate the new method by comparing it with a fully explicit code for compressible flow at general Mach numbers showing a good agreement in all quantities of interest. The differences between the results of the two codes are on the order of the square of the Mach number caused by the disregard of high-order terms in the Mach number in the new algorithm. The relative difference found for a specific low value of the Mach number of 0.05 is on the order of 1% for instantaneous and mean quantities of the two phases. We also quantify the efficiency of the new algorithm by comparing the computational time it takes to simulate one time unit with both codes.

4.1 Introduction

Multiphase flows with a large number of droplets dispersed into a gas play an important role in a variety of technological applications and environmental problems. Examples include thermal processing in food manufacturing, air pollution control and heat transfer in power stations (Barigou et al. 1998). In this paper we investigate a coupled Euler-Lagrange model to simulate droplet-laden turbulent channel flow in which phase transition plays an important role. The first such Euler-Lagrange study of mass and heat transfer in droplet-laden turbulent flow was done by Mashayek in 1998 (Mashayek 1998). He conducted a simulation study, investigating homogeneous turbulence with two-way coupling between the gas and the dis-

persed droplet phase involving momentum, mass and energy of the system. Later, a study dedicated to the mixing layer with embedded evaporating droplets was conducted by Miller and Bellan (1998). In Masi et al. (2010) a cloud of inertial evaporating droplets, interacting with a non-isothermal droplet-laden turbulent planar jet, is considered. In the present paper we present a new time-stepping algorithm tailored to compressible flow at low Mach numbers and extend the work of Mashayek (1998) to wall-bounded turbulence by investigating turbulent channel flow with a dispersed droplet phase undergoing phase transition. The models adopted here are identical to the models used in Miller and Bellan (1998) and Masi et al. (2010). The main difference between the current study and the studies mentioned above is that we consider conditions in which not only evaporation of droplets but also their growth by condensation of the vapor phase are important.

In this paper we consider fully developed turbulent channel flow of a mixture of air and water vapor in which water droplets are dispersed. Fully developed turbulent channel flow is treated as homogeneous in the streamwise and spanwise directions (Pope 2000) and therefore, periodic boundary conditions are used in these directions, as in Kim et al. (1987).

A turbulent flow can be modeled in various ways. In this paper we make use of direct numerical simulation in which all scales of the flow, except the detailed flow around each droplet, are resolved. The solution is time dependent and the time step is limited by both stability and accuracy considerations.

In this study the mixture of air and water vapor will be referred to as the carrier phase or the carrier gas and the droplets as the dispersed phase. Incorporation of evaporation and condensation of the dispersed phase raises the question whether or not to include explicit compressibility of the carrier phase. If the carrier gas is assumed to be strictly incompressible then the inclusion of evaporation and condensation is subject to the condition that all instantaneous changes in the local mass density of air and water vapor cancel each other precisely throughout the domain. A full simulation model can be developed for such an incompressible carrier phase (Russo et al. 2014). The incompressible treatment of the carrier phase would still permit to incorporate changes in mass density into the model using the equation of state and the Boussinesq approximation, which implies the dependence of mass density on temperature and vapor mass fraction. In our problem we relax the physical approximations further and allow the divergence of velocity not to be equal to zero as a result of phase transitions. This motivates us to treat the carrier phase as compressible flow which is characterized by a low Mach number, much smaller than 1 for the chosen initial conditions. The focus in this paper is on the development of a new low Mach number algorithm suitable for multiphase flow with phase transition, extending earlier work by Bell et al. (2004). This algorithm must be efficient for low Mach numbers: it should be possible to take a time step independent of Mach number as $Ma \rightarrow 0$.

There are two main numerical techniques for the treatment of compressible low Mach number flows: density-based methods and pressure-based methods. Two types of time-marching procedures are applied in density-based methods: explicit and implicit algorithms. Explicit density-based methods have a stability restriction, called Courant-Friedrichs-Lewy (CFL) condition (Morton and Mayers 2005), which makes these algorithms computationally expensive at low Mach numbers. Our previous study of turbulent droplet-laden channel flow with phase transition was done with a density-based explicit time integration method (Bukhovstova et al. 2014a), which was restricted to values of the Mach number higher than the realistic value of 0.005. In implicit density-based methods the system of governing equations for compressible turbulent flow is ill-conditioned making iterative solutions excessively time

consuming (Roller and Munz 2000). In order to avoid this poor condition of the numerical problem two types of schemes are used in density-based methods: preconditioning (Tukel 1987) and asymptotic schemes (Müller 1998). The proposed techniques are only applicable to time-independent problems. In the present study all quantities are time dependent because of the turbulent flow and the phase transitions that occur.

In order to apply preconditioning to time-dependent problems the dual-time-stepping technique is normally used (Lessani 2003). The dual time-step method could also be considered for the actual compressible equations, facing the challenge of resolving very fast acoustic signals at low Mach numbers. We selected a different path and focus on the low Mach number approximation obtained as a result of asymptotic analysis and some approximations. The resulting system of equations is treated with a hybrid time stepping method. The approximated system has as virtue the absence of large eigenvalues which allows to adopt most of the terms explicitly. We closely follow the work of Bell et al. (2004) and extend this to multiphase problems.

Pressure-based methods are extensions of pressure correction methods used in incompressible flow (Fletcher (1988), Karki and Patankar (1989)). In incompressible flow the pressure correction follows from a Poisson equation which is obtained from the condition that the velocity field has zero divergence. In case of compressible low Mach number flow this divergence-free constraint on the velocity field is not applicable. In order to obtain a Poisson equation for the pressure an expression for the divergence of velocity is derived employing the continuity equation and the equation of state (Vreman et al. (2009), Bell et al. (2004)).

To obtain a suitable time integration method for the problem of droplet-laden turbulent channel flow we first perform a perturbation analysis in powers of the Mach number of the governing system of equations. An asymptotic analysis of the Navier-Stokes equations for this regime of flow conditions was conducted before in the study by Zank and Matthaeus (1991). They derived low Mach number equations from the compressible Navier-Stokes equations employing multiple time- and space-scale expansions in powers of the Mach number. The single time-scale and multiple space-scale analysis conducted by Klein (1995) gives insight into the low Mach number Euler equations. In this paper we use a multiple time scale, single space scale low Mach asymptotic analysis closely following Müller (1998) and later work of Boger et al. (2012). This approach allows to distinguish advective and acoustic modes for turbulent flows at low Mach numbers (Ristorcelli 1997). We take into account the lowest-order terms in Mach number and get a simplified system of governing equations applicable to a compressible carrier phase at low Mach numbers. The specific feature of this new system is the decomposition of pressure into two parts, one of which is independent of the spatial coordinates. This part of pressure is connected with other thermodynamic quantities through the equation of state. Another part can be called the 'incompressible' pressure since it only enters the velocity equation similarly to the pressure in the incompressible formulation. The obtained splitting of pressure motivates us to use a pressure-based method. Based on the decomposed pressure, we propose a time integration algorithm extending Bell et al. (2004) to the case of turbulent channel flow with water droplets which can undergo phase transition. This method also belongs to pressure-correction methods and we apply the continuity equation, the equation of state and the boundary conditions for the velocity in order to derive an expression for the divergence of velocity which will determine the pressure correction term. We validate the new numerical method by comparison with results obtained with the fully explicit code in Bukhovostova et al. (2014a). Statistical results, averaged in time and over the homogeneous directions, from both codes will be compared along with instantaneous quan-

tities. We will quantify the accuracy of the new method first and then the gain in computing time by comparing the time it takes to simulate one time unit with the two methods.

The organization of the paper is as follows. In section 4.2 we will present the mathematical model used in both codes. Next we describe in detail the low Mach number model in section 4.3. In section 4.4 the numerical method of the low Mach number algorithm is given. Results are presented in section 4.5 and concluding remarks are collected in section 4.6.

4.2 Governing equations for the gas-droplets system

This section is dedicated to the mathematical model which is the starting point of both the explicit numerical method and the low Mach number algorithm. First, general aspects of the problem and the geometry will be described along with the applied boundary conditions. Subsequently, the set of partial differential equations for the carrier phase, i.e., the gas consisting of air and water vapor, the system of ordinary differential equations for the dispersed phase and the source terms describing the coupling between the two phases will be presented in separate subsections.

4.2.1 *The description of the flow domain*

We consider a water-air system in a channel, bounded by two parallel horizontal plates. This is a two-phase system, consisting of a carrier phase and a dispersed phase, consisting of liquid water droplets. The carrier phase is considered using the Eulerian approach while the dispersed phase is treated in the Lagrangian manner.

In Figure 4.1 a sketch of the flow domain is presented. The domain has a size of $4\pi H$ in the streamwise direction, which is denoted by x , and $2\pi H$ in the spanwise direction, z , where H is half the channel height. In addition, y is the coordinate in the wall-normal direction. The total volume of the domain is defined by V . The top wall of the channel is denoted by $y = H$ and the bottom wall by $y = -H$. Studies done by Kim et al. (1987) motivate us to use periodic boundary conditions in the streamwise and spanwise directions. In addition, no-slip conditions are enforced for the carrier phase at the walls. A constant heat flux $\dot{Q}$ is applied through the walls: this heat flux is positive through the top wall and negative through the bottom wall. The flux at both walls is equal in size in order to conserve the total energy of the system.

4.2.2 *The governing equations*

The carrier gas is treated in the Eulerian manner as a compressible Newtonian fluid. We impose conservation of mass, momentum, total energy and water vapor. The equations can be written as Miller and Bellan (1998):

Fig. 4.1: The computational domain

$$\partial_t \rho + \partial_j (\rho u_j) = Q_m \quad (4.1)$$

$$\partial_t (\rho u_i) + \partial_j (\rho u_i u_j) = -\partial_j \pi_{ij} + F_i + Q_{mom,i} \quad (4.2)$$

$$\partial_t e_t + \partial_j (\rho u_j e_t) = -\partial_j q_j - \partial_j (u_i \pi_{ij}) + Q_e \quad (4.3)$$

$$\partial_t (\rho Y_v) + \partial_j (\rho u_j Y_v) = -\partial_j \phi_{v,j} + Q_m \quad (4.4)$$

where $Q_m, Q_{mom,i}, Q_e$ are sink/source terms expressing the two-way coupling between the phases. These will be described later. In addition, (ρ, u_j, e_t, Y_v) are the carrier phase mass density, components of the velocity, total energy density and vapor mass fraction, respectively. Moreover, π_{ij} denotes pressure and viscous contributions to the momentum flux. The term F_i is an external force density which is obtained from the conservation of total streamwise momentum. In addition, q_j denotes the components of the heat flux vector, which consists of heat transport by conduction and by diffusion and the vector ϕ_v defines the diffusive mass flux of water vapor. The pressure and temperature of the carrier phase are denoted by p and T . Moreover, Y_v, p and T are connected by the ideal gas law for an air-water vapor mixture. The dispersed phase is modeled using a point-particle approach following Miller and Bellan (1998) and Masi et al. (2010). We solve a system of ordinary differential equations in order to find position, velocity, temperature and mass of each single droplet, $\mathbf{w}_{drop} = [\mathbf{x}_i, \mathbf{v}_i, T_i, m_i]$ of the form:

$$\frac{d\mathbf{w}_{drop}}{dt} = N_{drop} \quad (4.5)$$

All details of this model can be found in Bukhvostova et al. (2014a).

The interaction between the two phases is modeled by the two-way coupling terms which are derived from the conservation of the total mass, momentum, energy and water mass of the system. For instance, the two-way coupling term Q_m follows from the conservation of the total mass in the system and equals:

$$Q_m = -\sum_i \frac{dm_i}{dt} \delta(\mathbf{x} - \mathbf{x}_i) \quad (4.6)$$

where the sum is taken over all droplets in the domain. The expressions for the other two-way coupling terms can be found in Bukhvostova et al. (2014a).

In the next section the need for a new numerical algorithm will be clarified and the mathematical model for low Mach number flow will be derived.

4.3 Low Mach number model

In this section the low Mach number model will be presented. In subsection 4.1 we will motivate the need for a new numerical algorithm. Next, in subsection 4.2, we will describe the procedure of non-dimensionalization of the governing equations in this model. Subsection 4.3 is dedicated to the asymptotic analysis in powers of Mach number. Finally, in subsection 4.4 we describe the solution procedure for the new system of equations.

4.3.1 Motivation for the new model

In order to understand better the presence of fast scales which restrict the time step in a fully explicit method, we consider the system of equations (4.1)-(4.4) in 1D for simplicity. The eigenvalues of the Jacobian matrix of this system are: $\lambda_{1,2} = u$, $\lambda_3 = u + c$ and $\lambda_4 = u - c$ where c stands for the speed of sound. If the Mach number is small, these eigenvalues define two types of time scales present in the system: the long time the flow takes to travel one length scale with the velocity u and the short time it takes for an acoustic wave to travel this length scale. Further in the text these time scales will be referred to as fast and slow scales, respectively.

In explicit numerical methods for advection-diffusion equations the restriction on the time step according to the CFL condition is given by Morton and Mayers (2005):

$$\Delta t \leq \text{CFL} \times \min \left\{ \frac{\Delta x}{|\lambda_1|}, \frac{\Delta x}{|\lambda_2|}, \frac{\Delta x}{|\lambda_3|} \right\} \quad (4.7)$$

where Δx is the grid spacing. We conclude that the upper bound for the time step is proportional to $\Delta x/(u \pm c)$ which is approximated by $\Delta x/c$ because we deal with a low Mach number flow. Consequently, the non-dimensional time-step is bounded by $\text{CFL} \frac{\Delta x}{c} = \text{CFL} \frac{\Delta x}{u} \frac{u}{c} = \text{CFL} \text{Ma} \frac{\Delta x}{u}$, where the grid spacing Δx and the corresponding velocity component u are non-

dimensional. From a stability analysis of the Runge-Kutta method we found that in the explicit code $CFL = 2$ can be used. Consequently, the time-step which we can allow tends to zero when the Mach number tends to zero. This makes an explicit time integration computationally expensive for low Mach number flows.

It is known that for values of the Mach number up to 0.3 the fluid mechanics of single-phase turbulent channel flow corresponds well to that of incompressible flow (Anderson (2007), Russo et al. (2014)). However, there are three main differences between compressible and incompressible flows which can become more pronounced in case of multiphase flow with phase transitions. The characteristics of incompressible flow which are different from compressible flow are the following: a constant mass density, a zero divergence of the velocity and an infinite speed of sound. In this study compressibility appears because of changes in the mass density due to phase transitions, i.e., liquid water from the dispersed water droplets contributes to the vapor present in the carrier phase and vice versa. This apparent compressibility is expressed by a non-zero divergence of velocity and a non-zero gradient of the mass density. If we would treat the carrier phase of the current problem as incompressible we could still incorporate changes in mass density into the model using the equation of state and the Boussinesq approximation, which implies a dependence of mass density on temperature and vapor mass fraction. However, in such an approximation the non-zero divergence of velocity is not taken into account. In Bukhvostova et al. (2014a) we quantified the explicit compressibility comparing the RMS of the term $\rho \nabla \cdot \mathbf{u}$ with the RMS of the term $\mathbf{u} \cdot \nabla \rho$ in the continuity equation. It was shown that the RMS of these two terms has the same order of magnitude. In addition, we observe a significant difference in the heat transfer characteristics of the system during the initial stages caused by a net transfer of gas when the temperature gradient develops. Therefore, we consider the carrier phase as compressible and develop a suitable numerical treatment.

4.3.2 Non-dimensionalization procedure

In order to eliminate stability problems related to fast time scales we replace some of the variables in the system of equations by variables which only change on the slow time scale and solve the Navier-Stokes equation partially implicitly, i.e. the pressure term is considered using implicit time-stepping. In particular, we solve the temperature equation instead of total energy density equation (4.3) and the vapor mass fraction equation instead of the vapor mass density equation (4.4):

$$\begin{aligned} \rho (c_{pa} + Y_v(c_{pv} - c_{pa}))(\partial_t T + u_j \partial_j T) = & \partial_j(K(T) \partial_j T) + \\ & \partial_j(\rho D \partial_j Y_v((c_{pv} - c_{pa})T + \lambda_0)) + \mu(T) S_{ij} \partial_j u_i - \\ & (\lambda_0 + (c_{vv} - c_{va})T) \partial_j \rho D(T) \partial_j Y_v + Q_{temp} + \frac{Dp}{Dt} \end{aligned} \quad (4.8)$$

$$\partial_t Y_v + u_j \partial_j Y_v = \frac{1}{\rho} \partial_j(\rho D(T) \partial_j Y_v) + Q_{vapor} \quad (4.9)$$

where Q_{temp} and Q_{vapor} are two-way coupling terms which are given by:

$$Q_{vapor} = \frac{Q_m(1 - Y_v)}{\rho} \quad (4.10)$$

$$Q_{temp} = Q_e - u_i Q_{mom,i} - Q_m c_{vv} T + \frac{u_i^2 Q_m}{2} - Q_m \lambda_0 \quad (4.11)$$

The convective part of the vapor mass fraction equation is decoupled from the temperature and mass density equation (4.1) as can be seen in (4.9). Therefore, this equation only gives a diagonal term equal to u in the Jacobian matrix. The inviscid part of temperature equation (4.8) contains $u_j \partial_j T$ and $\frac{Dp}{Dt}$. The same reasoning as applied to the term $u_j \partial_j Y_v$ in (4.9) shows that $u_j \partial_j T$ does not introduce fast time scales into (4.8). The change of pressure, $\frac{Dp}{Dt}$, is also a slow process and does not bring fast scales into temperature equation (4.8). This will be clarified at the end of this section.

In order to make the system of governing equations non-dimensional we closely follow the procedure proposed by Müller (1998) and choose the following reference scales: ρ_{ref} , p_{ref} , u_{ref} , T_{ref} , μ_{ref} , k_{ref} , L_{ref} , $\mathcal{D}_{ref}$ which are the reference mass density, pressure, velocity, temperature, dynamic viscosity, thermal conductivity, length and mass diffusivity. The reference scales are chosen exactly in the way in which Müller (1998) does it: this choice guarantees that non-dimensional flow quantities remain of $\mathcal{O}(1)$ for any low reference Mach number which is equal to:

$$Ma = \frac{u_{ref}}{\sqrt{\gamma p_{ref} / \rho_{ref}}} \quad (4.12)$$

The reference temperature and mass density are the initial mean gas temperature and mass density, respectively. The reference length is chosen as half the channel height H . The velocity scale u_{ref} is taken as the initial bulk velocity of the carrier gas u_b . All other reference scales are defined by the initial conditions which are described in subsection 4.5.1. As a result of non-dimensionalization, we obtain the following system of non-dimensional equations:

$$\partial_t \rho + \partial_j (\rho u_j) = Q_m \quad (4.13)$$

$$\partial_t u_k + u_j \partial_j u_k + \frac{1}{\gamma Ma^2 \rho} \partial_k p = G_k + Q_{vel,k} \quad (4.14)$$

$$\partial_t T + u_j \partial_j T = \frac{E_T + \frac{\gamma-1}{\gamma} \frac{Dp_0}{Dt}}{\rho c_m} \quad (4.15)$$

$$\partial_t Y_v + u_j \partial_j Y_v = J_v + Q_{vapor} \quad (4.16)$$

In (4.14) $Q_{vel,k}$ stands for the coupling term in the velocity equation and it is equal to the following:

$$Q_{vel,k} = \frac{Q_{mom,k}}{\rho} - u_k \frac{Q_m}{\rho}. \quad (4.17)$$

The non-dimensional equation of state is:

$$p = \rho T (1 + M Y_v) \quad (4.18)$$

with $M = \frac{M_{air}}{M_{water}} - 1$ where M_{air} and M_{water} are the molar masses of pure air and water, respectively. Furthermore,

$$G_k = \frac{1}{\text{Re}_b \rho} \partial_j (\mu(T) S_{kj}) + \frac{1}{\rho} F_k \quad (4.19)$$

where Re_b stands for the bulk Reynolds number based on the bulk velocity. Moreover, E_T in non-dimensional temperature equation (4.15) is a complex expression which includes the two-way coupling term Q_{temp} :

$$E_T = \frac{1}{\text{PrRe}_b} \partial_j (\mu(T) \partial_j T) + \frac{1}{\text{ScRe}_b} \partial_j \mu(T) \left(\partial_j Y_v ((R-1)T + \lambda) \right) + \quad (4.20)$$

$$\frac{(\gamma-1)\text{Ma}^2}{\text{Re}_b} \mu(T) S_{ij} \partial_j u_i - \frac{1}{\text{ScRe}_b} \left(\lambda + \left[\frac{R}{\gamma_{vapor}} - \frac{1}{\gamma} \right] T \right) \partial_j \mu(T) \partial_j Y_v +$$

$$(\gamma-1)\text{Ma}^2 Q_{temp}$$

where Pr, Sc denote the Prandtl number and the Schmidt number, respectively. Finally, γ_{vapor} and γ are the ratio of specific heats for water vapor and air, respectively, and $c_m = Y_v(R-1) + 1$ with $R = \frac{c_{pv}}{c_{pa}}$. The five terms on the right-hand side of (4.20) correspond to the five terms on the right-hand side of dimensional temperature equation (4.15). The pressure derivative term is written separately for convenience of the further derivation.

In the non-dimensional vapor mass fraction equation J_v stands for:

$$J_v = \frac{1}{\rho \text{Re}_b \text{Sc}} \partial_j \mu(T) \partial_j Y_v \quad (4.21)$$

4.3.3 Asymptotic analysis

Since we only consider the low Mach number equations and ignore the fast acoustic time scale and since the governing equations only depend on the Mach number through Ma^2 , we can follow Boger et al. (2012) and use an expansion of all quantities in powers of Ma^2 , e.g.:

$$p(\mathbf{x}, t, \text{Ma}) = p_0(\mathbf{x}, t) + \text{Ma}^2 p_2(\mathbf{x}, t) + \text{Ma}^4 p_4(\mathbf{x}, t) + O(\text{Ma}^6) \quad (4.22)$$

As a result of the choice of the reference scales, p_0, p_2, p_4 etc., in these expansions do not depend on the Mach number (Müller 1998). We substitute all expansions in the system of governing equations (4.13)-(4.16) and (4.18). As a result we obtain the zeroth-order continuity equation:

$$\partial_t \rho_0 + \partial_j (\rho u_j)_0 = Q_{m,0} \quad (4.23)$$

Subscripts 0 in Q_m and all other expressions below indicate that the zeroth order expansion functions in the expressions of the form (4.22) enter these terms.

The leading momentum equations are the following:

$$\partial_j p_0 = 0 \quad (4.24)$$

$$\partial_t u_{k,0} + u_{k,0} \partial_j u_{k,0} + \frac{1}{\gamma p_0} \partial_k p_2 = G_{k,0} + Q_{vel,k,0} \quad (4.25)$$

The leading temperature and vapor mass fraction equations are:

$$\partial_t T_0 + u_{j,0} \partial_j T_0 = \frac{E_{T,0} + \frac{\gamma-1}{\gamma} \frac{Dp_0}{Dt}}{\rho_0 c_{m,0}} \quad (4.26)$$

$$\partial_t Y_{v,0} + u_{j,0} \partial_j Y_{v,0} = J_{v,0} + Q_{vapor,0} \quad (4.27)$$

Equations (4.23), (4.24), (4.25), (4.26), (4.27) form the final system of the governing equations together with the equation of state obtained from the asymptotic analysis:

$$p_0 = \rho_0 T_0 (1 + MY_{v,0}) \quad (4.28)$$

For sake of simplicity, in the following the subscript 0 will be omitted in all variables except p_0 .

4.3.4 Solution procedure

The solution procedure for the system of equations (4.23)-(4.28) consists of three major steps: first, finding the gas temperature and the vapor fraction at the new stage, second, finding the gas density and p_0 and third, finding the gas velocity. The first two steps are described in the text below along with the expressions for the divergence of the velocity field and the expression for $\frac{Dp_0}{Dt}$. The procedure for the velocity is an extension of the pressure-correction method and will be discussed in Section 4.4.1. The temperature and vapor mass fraction equations, (4.26) and (4.27), can be solved explicitly as there are no fast time scales in these equations. The coupled equations for mass density and velocity of the carrier phase, (4.23) and (4.25), still contain both small and large eigenvalues. In order to avoid the time step restriction we follow an alternative strategy which is outlined next.

A special procedure is applied to find the mass density of the carrier phase. The mass density can be calculated from equation of state (4.28) if apart from temperature and vapor mass fraction also p_0 would be known. In order to find p_0 we integrate (4.23) over the total computational domain V and obtain the total mass, m . We find an expression for the mass density from (4.28) and integrate it over the computational domain in order to find m using the independence of p_0 on the spatial coordinates. As a result we obtain the following expression in which m , T and Y_v are known at the new time level:

$$m = p_0 \int_V \frac{dV}{T(1 + MY_v)} \quad (4.29)$$

From (4.29) we find p_0 and subsequently the mass density is obtained from (4.28).

For the update of the carrier gas velocity we apply an extension of the pressure-correction procedure usually applied to incompressible flows (Fletcher 1988). It consists of three steps. First, a so-called 'provisional' velocity from the Navier-Stokes equation, based on velocity, density, temperature and pressure from the previous time is calculated. This velocity does not satisfy the correct criterion for its divergence which in case of incompressible flow is $\nabla \cdot \mathbf{u} = 0$. In order to correct the provisional velocity a Poisson equation for the pressure is solved during the second step. Finally, in the third step the provisional velocity is corrected

with this pressure such that the correct divergence of velocity is obtained.

To find the divergence of velocity we start with the expression for the material derivative of p_0 following Bell et al. (2004), using equation of state (4.28):

$$\frac{Dp_0}{Dt} = \frac{\partial p_0}{\partial \rho} \frac{D\rho}{Dt} + \frac{\partial p_0}{\partial T} \frac{DT}{Dt} + \frac{\partial p_0}{\partial Y_v} \frac{DY_v}{Dt} \quad (4.30)$$

Next, we substitute into the right-hand side of (4.30) the material derivatives $\frac{D\rho}{Dt}$, $\frac{DT}{Dt}$ and $\frac{DY_v}{Dt}$ from the governing equations (4.23), (4.26), (4.27). All partial derivatives on the right-hand side of (4.30) follow from (4.28). After substitution of all terms on the right-hand side of (4.30) we obtain:

$$\nabla \cdot \mathbf{u} = -\frac{1}{p_0} \frac{Dp_0}{Dt} + \frac{Q_m}{\rho} + \frac{1}{T\rho c_m} \left(E_T + \frac{\gamma-1}{\gamma} \frac{Dp_0}{Dt} \right) + \frac{M}{1+Y_v M} \left(J_v + Q_{vapor} \right) \quad (4.31)$$

Since $\frac{Dp_0}{Dt}$ in (4.31) is not known, we integrate (4.31) over the total computational domain. Using the boundary conditions for the velocity, i.e. no-slip boundary conditions at the walls of the channel and periodic boundary conditions in the stream- and spanwise directions, we obtain that $\int_V \nabla \cdot \mathbf{u} = 0$. Using the independence of p_0 of the spatial coordinates, we get:

$$\frac{Dp_0}{Dt} = \frac{\int_V \left[\frac{Q_m}{\rho} + \frac{E_T}{T c_m \rho} + \frac{M}{1+MY_v} (J_v + Q_{vapor}) \right] dV}{\frac{V}{p_0} - \frac{\gamma-1}{\gamma} \int_V \frac{dV}{T c_m \rho}} \quad (4.32)$$

Finally, we find the divergence of the velocity from (4.31). Note that expression (4.31) is obtained applying the specific conditions for the velocity at the boundary.

Expression (4.32) is also used in temperature equation (4.26). Since p_0 is independent of the spatial coordinates, the material derivative of p_0 is equal to $\frac{\partial p_0}{\partial t}$. We investigated the change in time of p_0 calculated from (4.29) and of temperature calculated with the explicit code. In the middle of the channel the relative change in temperature is 10^4 times larger than the relative change in p_0 . It means that the change of p_0 in time is a slow process and does not introduce large eigenvalues in temperature equation (4.26).

The forcing terms in the velocity, temperature and vapor mass fraction equations are derived from the conditions of constant momentum in all directions, constant total energy of the system and constant water vapor mass, respectively. This finishes the description of the low Mach number model. In the next section the numerical method for this model will be discussed.

4.4 Numerical method

The numerical method for the low Mach number model will be presented here. First, the details on the time integration algorithm will be given. Second, we will discuss the spatial discretization along with the boundary conditions and we will derive the Poisson equation for pressure and specify the method used for its solution.

4.4.1 Time integration algorithm

Since the term $-\frac{1}{\gamma p}\partial_k p_2$ in velocity equation (4.25) introduces large eigenvalues, we need to treat this term in an implicit way. The system of governing equations for the carrier phase (4.23), (4.25), (4.26) and (4.27) is written in the following way for the vector of unknowns $\mathbf{w} = [\rho, u_i, T, Y_v]$; the linear part consists only of the pressure term in the velocity equation:

$$\frac{\partial \mathbf{w}}{\partial t} = L(\mathbf{w}) + N(\mathbf{w}), \quad (4.33)$$

where L and N are linear and nonlinear operators, correspondingly, given by:

$$N(\mathbf{w}) = \begin{pmatrix} -\partial_j(\rho u_j) + Q_m \\ -u_j \partial_j u_i + \frac{1}{\rho} \partial_j(\mu(T) S_{ij}) + \frac{1}{\rho} F_i + Q_{vel,i} \\ -u_j \partial_j T + \frac{E + \frac{D_p}{D_t} + S_T}{\rho(c_{pa} + Y_v(c_{pv} - c_{pa}))} \\ -u_j \partial_j Y_v + \frac{J_v}{\rho} + Q_{vapor} \end{pmatrix}$$

and

$$L(\mathbf{w}) = \begin{pmatrix} 0 \\ -\frac{1}{\rho} \partial_i p_2 \\ 0 \\ 0 \end{pmatrix}.$$

There are not so many hybrid implicit-explicit time integration methods. We use the method proposed by Spalart et. al (1991), which is a three-stage low-storage Runge-Kutta scheme of highest possible order. For the nonlinear part N each stage is analogous to forward Euler or second-order Adams-Bashforth but with different coefficients γ and ζ . For the linear part L the method is similar to the Crank-Nicolson scheme but again with different coefficients. The hybrid scheme in which the pressure term is solved implicitly is second-order accurate in time.

The solution at $t + \Delta t$, $\mathbf{w}^{n+1}$, is found in three substeps starting from $\mathbf{w}^n$ at time t :

$$\mathbf{w}^{(1)} = \mathbf{w}^{(0)} + \Delta t \left[L(\alpha_1 \mathbf{w}^{(0)} + \beta_1 \mathbf{w}^{(1)}) + \gamma_1 N^{(0)} \right] \quad (4.34)$$

$$\mathbf{w}^{(2)} = \mathbf{w}^{(1)} + \Delta t [L(\alpha_2 \mathbf{w}^{(1)} + \beta_2 \mathbf{w}^{(2)}) + \gamma_2 N^{(1)} + \zeta_1 N^{(0)}] \quad (4.35)$$

$$\mathbf{w}^{(3)} = \mathbf{w}^{(2)} + \Delta t [L(\alpha_3 \mathbf{w}^{(2)} + \beta_3 \mathbf{w}^{(3)}) + \gamma_3 N^{(2)} + \zeta_2 N^{(1)}] \quad (4.36)$$

where $\mathbf{w}^{(n)} = \mathbf{w}^{(0)}$ and $\mathbf{w}^{(n+1)} = \mathbf{w}^{(3)}$ with the following values of the coefficients:

$$\begin{aligned} \gamma_1 &= \frac{8}{15}, & \gamma_2 &= \frac{5}{12}, & \gamma_3 &= \frac{3}{4}, & \zeta_1 &= -\frac{17}{60}, & \zeta_2 &= -\frac{5}{12}, \\ & & & & \alpha_1 &= \frac{29}{96}, & \alpha_2 &= -\frac{3}{40}, & \alpha_3 &= \frac{1}{6}, \\ & & & & \beta_1 &= \frac{37}{160}, & \beta_2 &= \frac{5}{24}, & \beta_3 &= \frac{1}{6}, \end{aligned}$$

which were obtained from the condition of highest possible order of the algorithm.

We do not solve all the quantities simultaneously. The following order is used during each stage of the time step. First, we solve the system of equations for the dispersed phase explicitly using droplet and gas values at the previous stage. The right-hand sides of the droplet equations contain gas properties at the droplet location. In order to determine these, tri-linear interpolation is applied (Marchioli et al. 2008). From the droplet properties at the new stage we also obtain the two-way coupling terms at this time. Next, we solve the system of equations for the carrier phase: first, we find the temperature and vapor mass fraction at the new stage, next the mass density and finally the velocity. The temperature and the vapor mass fraction equations are solved explicitly. Following the procedure for the mass density, described in the previous section, we find p_0 and the mass density by calculating the total mass in the computational domain, m , in an explicit way.

For the velocity we use an extension of the pressure-correction procedure for low Mach number compressible flows (Bell et al. 2004). First, we find a provisional velocity $\mathbf{u}^*$, using the velocity, density, temperature and gradient $\partial_j p_2$ from the previous stage, i.e., this velocity is found in an explicit way. This provisional velocity does not satisfy the requirement for the divergence of velocity found in (4.31). During the second step we find p_2 at the new stage from the Poisson equation:

$$\nabla \cdot \left(\frac{1}{\rho^{i+1}} \nabla p_2^{i+1} \right) = \frac{\nabla \cdot \mathbf{u}^* - \nabla \cdot \mathbf{u}^{i+1}}{\beta_{i+1} \Delta t}, \quad (4.37)$$

where $i = 0, 1, 2$. The expression for $\nabla \cdot \mathbf{u}^{i+1}$ is known from (4.31). It requires $\frac{Dp_0}{Dt}$, the temperature, the vapor fraction and the mass density at the new stage. In order to find $\frac{Dp_0}{Dt}$ at the new stage the new temperature, mass density, vapor mass fraction and p_0 are required according to (4.32). All these quantities were already obtained during the current stage of the time step, which makes it possible to calculate the right-hand side of Poisson equation (4.37) and, consequently, to solve it for the new pressure p_2^{i+1} .

During the third step of the pressure-correction procedure we apply p_2 to correct the velocity:

$$\mathbf{u}^{i+1} = \mathbf{u}^* - \Delta t \beta_{i+1} \frac{1}{\rho^{i+1}} \nabla p_2^{i+1} \quad (4.38)$$

In this way the new velocity $\mathbf{u}^{i+1}$ satisfies the requirement on the divergence, (4.31).

4.4.2 Spatial discretization

The spatial discretization is based on a finite volume method which closely follows the method in Bukhvostova et al. (2014a). The geometry is divided into rectangular cells. In the streamwise and spanwise directions a uniform grid is used, while in the wall-normal direction we apply a non-uniform grid which is finer near the walls in order to resolve the boundary layer. Throughout this paper n_x, n_z and n_y stand for the number of grid points in the streamwise, spanwise and wall-normal directions, respectively. The variables are stored in the centers of the cells. We use 128 grid points in all three directions. The choice of the grid resolution is motivated by Marchioli et al. (2008) where a similar mesh was used for a

finite-volume code and comparison with other methods and refinements established the degree of convergence of the solution.

The equations which we solve in the low Mach number model are not in conservative form. The treatment of the convective and viscous parts is shown for velocity equation (4.25). The pressure gradient is treated according to the pressure-correction procedure that was discussed above and the details on the spatial discretisation of the Poisson equation will be given later in this section. The convective term in (4.25) $u_j \partial_j u_i$ is written as: $\partial_j u_i u_j - u_i \partial_j u_j$. The term $\partial_j u_i u_j$ is computed using a finite-volume method. For the term $u_i \partial_j u_j$ we calculate $\partial_j u_j$ with a finite-volume method and we multiply it with the value of the corresponding velocity component at the cell-center. The term $\partial_j (\mu(T) S_{ij})$ is calculated applying a finite volume method and subsequently divided by the mass density ρ in the cell center. The viscous and convective terms of equations (4.26) and (4.27) are computed in a similar way.

4.4.3 Poisson equation

In the velocity equation (4.25) we do not need p_2 itself but the gradient of p_2 divided by the mass density. That is why we define a new scalar q given by:

$$\nabla q = \frac{1}{\rho} \nabla p_2 \quad (4.39)$$

Consequently, Poisson equation (4.37) can be rewritten as:

$$\Delta q = R, \quad (4.40)$$

where R denotes the right-hand side of the Poisson equation (4.37). The use of periodic boundary conditions in the homogeneous directions permits to perform a Fourier expansion of q in these directions and to apply an efficient solver for the Poisson equation. This approach is tailored to flows with two homogeneous directions and can not easily be extended to general configurations. The Fourier coefficients $\hat{q}_{k_x, k_z}$ depend on the wall-normal coordinate, where a pair (k_x, k_z) stands for a single Fourier mode and $0 \leq k_x \leq n_x/2$, $-n_z/2 \leq k_z \leq n_z/2$. We have a reduced number of modes in the streamwise direction because the Fourier transform of real data is such that: $\hat{q}_{-k_x, -k_z} = \hat{q}_{k_x, k_z}^*$ where $\hat{q}^*$ denotes the complex conjugate. The Fourier expansion in the two homogeneous directions for q is:

$$q(x, y, z) = \sum_{\substack{-n_x/2 \leq k_x \leq n_x/2, \\ -n_z/2 \leq k_z \leq n_z/2}} \hat{q}_{k_x, k_z}(y) \exp^{2\pi i \left(\frac{k_x x}{L_x} + \frac{k_z z}{L_z} \right)}, \quad (4.41)$$

where L_x and L_z stand for the size of the computational domain in the streamwise and spanwise directions, respectively. Substituting this expansion into (4.40) and performing a Fourier transform of R , we obtain:

$$\left(- \left(\frac{2\pi k_x}{L_x} \right)^2 - \left(\frac{2\pi k_z}{L_z} \right)^2 + \frac{d^2}{dy^2} \right) \hat{q}_{k_x, k_z} = \hat{R}_{k_x, k_z}, \quad (4.42)$$

where $\hat{R}_{k_x, k_z}$ denotes the Fourier coefficients of R . We approximate derivatives in the homogeneous directions by the derivative of the Fourier expansion.

In order to solve (4.42) we discretize the second derivative in the wall-normal direction of $\hat{q}_{k_x, k_z}$, using a five-point stencil with third-order accuracy on a non-uniform grid. On a uniform grid it becomes fourth-order accurate. As a result we obtain a linear system of equations of the form $A\hat{q}_{k_x, k_z} = \hat{R}_{k_x, k_z}$ for each pair (k_x, k_z) . The boundary conditions follow from the Navier-Stokes equation for the wall-normal velocity component, (4.25). Neglecting the viscous terms in this equation and applying no-slip boundary conditions to the velocity, we get $\frac{1}{\rho} \frac{\partial p_2}{\partial y} \Big|_{walls} = 0$ which is equivalent to $\frac{\partial q}{\partial y} \Big|_{walls} = 0$. We discretize these boundary conditions using a three-point stencil using one 'ghost' cell outside the geometry at each boundary. In order to have a unique solution of the Poisson equation we need to use at least one Dirichlet boundary condition for the mode $(k_x, k_z) = (0, 0)$. At the same time the Poisson equation must satisfy the compatibility condition for a solution to exist:

$$\int_{-H}^H \hat{R}_{k_x, k_z} dy = 0 \quad (4.43)$$

We use the Dirichlet condition at one wall and the Neumann boundary condition at the other. The Neumann condition at the first wall will be satisfied, since the compatibility condition is satisfied.

Solving $A\hat{q}_{k_x, k_z} = \hat{R}_{k_x, k_z}$ for each Fourier mode (k_x, k_z) using LU-decomposition of matrix A , we find $\hat{q}$ and, consequently, perform a back Fourier transform to find q . As was stated above, we do not need the pressure p_2 itself but in principle it can be computed from (4.39) by integration since ρ and q are both known.

In this study we use a collocated grid with variables stored in cell centers. The fluxes at the cell faces are found using linear interpolation of the corresponding quantities. This approach is known to lead to odd-even decoupling in some cases, resulting in oscillations in pressure and velocity fields. The solution for q and the wall-normal velocity component were found not to suffer from this effect with the current method, as is illustrated in Figure 4.2a and Figure 4.2b, which display smooth dependency of typical solution components on the spatial coordinates.

4.4.4 Boundary conditions

We apply periodic boundary conditions in the streamwise and spanwise directions for all variables. For the vapor mass fraction we use $\frac{\partial Y_v}{\partial y} \Big|_{walls} = 0$ in order to avoid diffusion of vapor through the walls. The boundary condition at the walls for the temperature of the carrier gas is found from the condition of constant heat flux to the walls, q_{wall} :

$$q_{wall} = -k(T) \frac{\partial T}{\partial y} \Big|_{walls} \quad (4.44)$$

Keeping q_{wall} constant we can find the wall-normal derivative of the temperature at the walls, using one 'ghost' point outside the geometry at each wall.

Fig. 4.2: (a) q (b) wall-normal velocity component on the characteristic line perpendicular to the channel walls as a function of the wall-normal coordinate y/H . Solid: $t = 0.1$ s, dashed: $t = 2$ s.

For the droplets periodic conditions are used in the homogeneous directions. This means that if a droplet leaves the domain, it re-enters the domain from the other side with the same properties. Moreover, droplets collide elastically with the walls if they approach the wall within a distance of their radius.

4.5 Validation of the method

This section consists of two parts: specification of the initial conditions for the simulations and presentation of the results. In the results part we will compare the results and efficiency of the low Mach number code with the explicit code, thereby establishing the accuracy of the expansion in the Mach number including zeroth order for all solution components apart from the pressure for which also the second-order term in the expansion is retained.

4.5.1 Initial conditions

In both codes the simulations are started from a turbulent velocity field, obtained from a simulation without droplets at the correct value of the Mach number with adiabatic boundary conditions. This simulation was done with the fully explicit code until the statistically steady state was reached in which the solution fluctuates around a well-defined mean state.

The developed numerical method can be applied to any initial conditions but since the results

from the fully explicit code are available we use the following initial condition: atmospheric pressure, room temperature and relative humidity equal to 100% which corresponds to one of the simulated cases in Bukhvostova et al. (2014a). The values of the thermodynamic parameters of the flow can be found in Bukhvostova et al. (2014a) for a mean temperature of 293.15 K. The initial conditions determine the non-dimensional parameters of the simulation are shown in Table 4.1.

The Mach number, $Ma = 0.05$, does not correspond to the reference velocity; the actual Mach number is ten times smaller. The motivation for the adopted value is CFL condition (4.7): at this Mach number the explicit code can be applied with an acceptable amount of computing time, thus providing a point of reference for the current new algorithm (Bukhvostova et al. 2014a). In Bukhvostova et al. (2014a) it was shown that for this Mach number the flow physics and heat and mass transfer characteristics are accurately approximated comparing results of the compressible formulation with those of an incompressible model.

In all results shown in this paper the initial conditions are chosen in the following way. For

Re_b	Pr	Ma	Sc
2333	0.7478	0.05	0.06283

Table 4.1: Non-dimensional parameters of the simulation

the explicit solver a snapshot of the solution in the statistically steady state was chosen of the same system of equations, but in the absence of droplets and with adiabatic boundary conditions. For the low Mach number solver the same initial velocity field was used, but the temperature and mass density were taken constant, corresponding to the solution of the system of equations (4.23)-(4.28) in the statistically steady state for adiabatic boundary conditions. The differences in the initial temperature between the two solvers are of order Ma^2 and can be seen in Figure 4.3. The initial vapor mass fraction is for both solvers found from the condition of 100% relative humidity.

This particular method for choosing the initial conditions for the low Mach number solver depends on the availability of an explicit solver. In order to avoid this restriction, we verified that the low Mach number solver can also be used to simulate the same flow starting from a laminar velocity profile onto which small two- and three-dimensional perturbations were superposed. Indeed, we found that the differences in statistical properties of the solutions arising from these two initial conditions are negligible.

We randomly distribute 2,000,000 droplets over the volume of the channel. The initial droplet diameter is given by $d_i/H = 3.09 \times 10^{-3}$. The initial droplet diameter satisfies the conditions for the point-particle approach (Bukhvostova et al. 2014a). The initial volume fraction of droplets is on the order of 10^{-4} . According to the classification in Elghobashi (1994) this fraction is high enough so that two-way coupling is required and low enough for the effects of collisions between droplets to be negligible. Velocity and temperature of the droplets are initialized using the carrier gas values at the droplet locations.

Fig. 4.3: Initial gas temperature averaged over the homogeneous directions as a function of the wall-normal coordinate. Solid: low Mach number code, dashed: explicit code.

4.5.2 Comparison of results from the two codes

Comparison of the results from the two algorithms, i.e., the explicit method and the hybrid approach, can be performed in two ways. For short times local, instantaneous results can be compared. For turbulent flow, however, small differences in initial conditions or in algorithms lead to large differences after a finite time. Therefore, instantaneous results cannot be compared over longer time intervals. In the turbulent regime with time-independent boundary conditions, the flow reaches a statistically steady state in which the solution fluctuates around a mean. The statistically steady state can be compared for both methods. The second method of validation is therefore based on a comparison of statistical quantities in this statistically steady state. Statistical results are obtained by averaging over the homogeneous directions and over time. Since the error in statistical quantities depends on the time interval used for averaging we can not expect smaller differences between the statistical results from the two solvers than this time-averaging error, which is estimated around 1% for the current simulation and averaging time (Vreman and Kuerten 2014). Throughout the paper quantities averaged over the homogeneous directions and over time will be denoted by brackets, $\langle \cdot \rangle$. Averaging over the homogeneous directions at a certain time is denoted by bars, $\bar{\cdot}$. All results are presented in non-dimensional units.

4.5.2.1 Instantaneous results

First, the time history of the streamwise and spanwise components of the gas velocity are compared in one point in the middle of the channel. Figures 4.4a and 4.4b show a close agreement in the velocity components even up to time 15, corresponding to $15H/u_b$ flow-

through times. Until this moment, the difference is on the order of 1%.

In the sequel differences in the results on the order of 1% will be referred to as close or good agreement. This order of difference is considered to be acceptable to conclude that the developed low Mach number model can be used for simulating turbulent droplet-laden channel flow with phase transitions.

Fig. 4.4: (a) Streamwise velocity component (b): Spanwise velocity component at point $(0.3H, 0.15H, 0)$ as a function of time. Solid: low Mach number code, dashed: explicit code.

4.5.2.2 Mean results

The carrier gas reaches a statistically steady state for which the mean profiles are determined after time $150H/u_b$. In Figure 4.5 the instantaneous temperature near the bottom wall is shown. We observe that after time $150H/u_b$ changes in the gas temperature are less than 1% with respect to the reference temperature; that condition was selected to start averaging from this time. The time averaging for all quantities is performed over the interval $[150H/u_b; 700H/u_b]$. Based on the statistical errors calculated in Vreman and Kuerten (2014) for a similar system we estimate that averaging over the chosen interval results in maximum statistical relative errors on the order of less than 1% in all quantities and to errors on the order of 1% in their RMS.

Figure 4.6 shows a good agreement between the low-Mach model and the fully compressible model in the mean temperature of the carrier phase and in the rms of the wall-normal component of the velocity. To quantify this agreement we calculate the relative difference which is equal to the L^2 -norm of the difference between the results of the two codes, divided by the L^2 -norm of the result of the low Mach number code:

$$\Delta = \frac{\sqrt{\sum_{k=1}^{n_y} (\langle u \rangle_k^{Mach} - \langle u \rangle_k^{expl})^2}}{\sqrt{\sum_{k=1}^{n_y} (\langle u \rangle_k^{Mach})^2}} \quad (4.45)$$

where the superscripts *Mach* and *expl* denote the low Mach number code and the explicit code, respectively. The relative difference Δ is below 3% for the rms of the wall-normal velocity for the time interval considered. Quantifying the difference between the results of the two codes in the gas mean temperature, it makes sense to divide it by the difference in the mean gas temperature between the two walls in the low Mach number code which is the quantity of interest for this problem. Calculating in this way, Δ is equal to 1% for the mean gas temperature.

We consider the Nusselt number to express the efficiency of the heat transfer between the channel walls. The Nusselt number is defined in the following way:

$$\text{Nu} = \left(\frac{dT_g}{dy} \Big|_{\text{wall}} \right) / \frac{\Delta T_g}{2H} \quad (4.46)$$

where ΔT_g is the difference in gas temperature between the two walls and the derivative with respect to the wall-normal coordinate in the numerator is the average over both walls. We compare the history of the Nusselt number in Figure 4.7, which shows a close agreement. The relative difference in the Nusselt number averaged in time over the steady state is equal to 0.1%. The droplet mean temperature in Figure 4.8 shows a good agreement between the two codes with a relative difference Δ equal to 3%. This difference is made non-dimensional using the difference in the mean droplet temperature between the two walls, found with the low Mach number method.

We also consider the droplet size probability density function (PDF) near the walls, Figure 4.9a and 4.9b. In order to compute this PDF, the wall-normal direction was divided into 64 equidistant slabs parallel to the channel walls. In each slab we distinguish 100 bins representing different diameter ranges distributed uniformly between $d_{\min}$ and $d_{\max}$ which are the minimum and maximum diameter among the droplets present in a certain slab. Next we compute for each slab the number of droplets within a certain bin. The size is normalized with the initial droplet diameter, d_0 . The figure shows a good agreement between the results of the two codes for this quantity. In order to verify that the differences between the two codes are on the order of Ma^2 we also performed the simulation with the two codes for $\text{Ma} = 0.1$, Figure 4.9c. In order to quantify the difference in the droplet size PDF in the two formulations we compute the L^2 -norm of the difference. We find that the norm of the differences between the results for $\text{Ma} = 0.1$ is four times larger than this norm for $\text{Ma} = 0.05$. This illustrates that the difference between the two methods is on the order of Ma^2 . The same result for the difference between the results of the two codes was found for the gas and droplet temperature averaged in time and in the homogeneous directions.

The comparison of the results of the two methods shows a good agreement: the differences in the kinematic and heat transfer properties along with the droplet characteristics are on the order of 1%. Next we will quantify the extent by which the new low Mach number method permits to simulate more efficiently than the explicit method at low Mach numbers.

4.5.2.3 Stability analysis and the time step

We performed a stability analysis for both the explicit method (4.1)-(4.4) and the low Mach number algorithm (4.23)-(4.28) in the same way as done by Müller and Rizzi (1987) for an

Fig. 4.5: Gas temperature at point $(0.3H, 0.15H, -0.012H)$ history in the low Mach number code.

Fig. 4.6: (a) Mean gas temperature and (b) RMS of the wall-normal gas velocity as a function of the wall-normal coordinate. Solid: low Mach number code, dashed: explicit code.

explicit algorithm for compressible, viscous flow. The stability analysis consists of two parts. First, the equations are linearized and discretized in space. This leads to a large system of coupled, linear ordinary differential equations. Fourier analysis results in a diagonal system of equations of the form:

$$\frac{d\mathbf{v}}{dt} = \Lambda \mathbf{v} \quad (4.47)$$

Fig. 4.7: Nusselt number history. Solid: low Mach number code, dashed: explicit code.

Fig. 4.8: Droplet mean temperature as function of the wall-normal coordinate. Solid: low Mach number code, dashed: explicit code.

where $\mathbf{v}$ represents the vector of amplitudes of the Fourier modes and Λ is a diagonal matrix which contains the complex eigenvalues, λ_i . Second, the regions in which $\lambda_i \Delta t$ is stable for the specific Runge-Kutta schemes used in this paper are determined.

Following Müller and Rizzi (1987) for our systems of equations, we find that the diffusive terms in the equations lead to:

Fig. 4.9: Droplet size PDF at time 300 for $Ma = 0.05$. (a): near the hot wall, (b): near the cold wall. (c): Droplet size PDF at time 300 near the cold wall for $Ma = 0.1$. Solid: low Mach number code, dashed: explicit code

$$\frac{-4}{Re_b Sc \Delta x^2} < \text{Re}(\lambda_i) < 0 \quad (4.48)$$

for both methods. For the explicit algorithm the convective terms lead to:

$$|\text{Im}(\lambda_i)| < \frac{u}{Ma \Delta x} \quad (4.49)$$

and for the low Mach number algorithm:

$$|\text{Im}(\lambda_i)| < \frac{u}{\Delta x} \quad (4.50)$$

where u is a typical value for the velocity and Δx the typical grid size.

Figure 4.10 shows the regions in which $\lambda_i \Delta t$ should be to obtain stability for both algorithms. It turns out that for the parameters used in our simulations the diffusive terms lead to the most severe restriction on the time step for the low Mach number algorithm, whereas the convective terms are most restrictive for the explicit method. The explicit method is stable if $\Delta t < \text{RK} \frac{\Delta x^2 \text{ReSc}}{4}$ with $\text{RK} = 2$ and $\Delta t \leq \text{CFL} \times \text{Ma} \frac{\Delta x}{u}$ with $\text{CFL} = 2$. For the low Mach number code the time step should satisfy $\Delta t < \text{RK} \frac{\Delta x^2 \text{ReSc}}{4}$ with $\text{RK} = 2$ and $\Delta t < \text{CFL} \times \text{Ma} \frac{\Delta x}{u}$ with $\text{CFL} = 1$. Substituting the non-dimensional parameters of the simulation $\text{Re}_b = 2333$, $\text{Sc} = 0.632799$ and $\Delta x = 0.004$, we obtain as time step limits 0.01 in the low Mach number code and 0.0004 in the explicit code.

We notice from the above restrictions on the time step in the low Mach number solver that the relevant bounds do not depend on the Mach number. As a result, we can simulate flows at different small Mach numbers with the same time step. This big advantage of the low Mach number method can also be shown analytically. As a result of making the system of governing equations for the carrier gas non-dimensional the Mach number is present in the temperature equation (4.26) only. In fact, the third and fifth terms on the right-hand side of (4.26) depend explicitly on the Mach number. It follows that the sum of the Mach number dependent terms in (4.26) is of order 1 with corrections which are of second order in the Mach number. Consequently, if the Mach number goes to zero, the dependence of the temperature equation on Mach number vanishes and, consequently, the system of governing equations does not depend on the Mach number. As a result, we can simulate flows at different small Mach numbers with the same time step. This was separately verified by performing simulations for three different small values of the Mach number, $\text{Ma}_1 = 0.005$, $\text{Ma}_2 = 0.025$ and $\text{Ma}_3 = 0.05$, using the maximum possible time step in the low Mach number code of 0.01. Knowing that the changes in the gas temperature are of order Ma^2 , $T(\text{Ma}) = T(0) + \alpha \text{Ma}^2 + \dots$, with constant α we expect:

$$R_{\text{Ma}} = \frac{T(\text{Ma}_3) - T(\text{Ma}_1)}{T(\text{Ma}_2) - T(\text{Ma}_1)} = 4.125 \quad (4.51)$$

Figure 4.11 shows that the difference $4.125 \times (T(\text{Ma}_2) - T(\text{Ma}_1))$ and $T(\text{Ma}_3) - T(\text{Ma}_1)$ are in close agreement at the arbitrary chosen point $(0.3H, 0.15H, -0.012H)$. We also plotted the difference $(T(\text{Ma}_3) - T(\text{Ma}_1)) - (T(\text{Ma}_2) - T(\text{Ma}_1)) \times 4.125$ which has a magnitude of 10^{-8} .

4.5.3 Computational efficiency

In the previous subsection the optimal time steps for the two solvers were determined. For the chosen grid and $\text{Ma} = 0.05$ the time step in the explicit solver has to be approximately 25 times smaller than the time step in the low Mach number solver.

We found that one time step with either method requires approximately the same CPU time on the same computer. A realistic Mach number, which in our test case is equal to 0.005,

Fig. 4.10: The outer bound of the stability region for solid: explicit solver, dashed: low Mach number solver. The figure shows the region in which the amplification factor of the scheme is smaller than 1.

would require a further reduction in the time step by a factor of ten in the explicit code. In the low Mach number code there is no need to decrease the time step because of its independence on the Mach number, as discussed in the previous subsection. Consequently, we may conclude that the problem considered here can be simulated approximately 250 times faster with the new numerical method than with the fully explicit code for the realistic small value of the Mach number.

Finally, we verified that using a 25 times larger time step in the low Mach number solver, compared to the explicit method at $Ma = 0.05$, yields deviations less than 1% in mean quantities such as gas velocity and temperature. This shows that the larger time step for the low Mach number solver is adequate for obtaining accurate results even though the asymptotic low Mach number analysis is adopted at this relatively high Mach number.

4.6 Conclusions

In this paper a new numerical approach for simulating droplet-laden turbulent channel flow with phase transitions at low Mach numbers was proposed. It is based on an asymptotic analysis at low Mach numbers. This numerical approach is beneficial because it avoids the dependence of the time step on Mach number arising from a CFL constraint on the time step in explicit time integration methods for low Mach numbers.

Results from the new low Mach number code were compared with results of a fully explicit code. We observe a good agreement in local instantaneous quantities along with a good agreement in mean quantities for both phases. The relative difference is equal to 1% in the

Fig. 4.11: Solid: $4.125 \times (T(\text{Ma}_2) - T(\text{Ma}_1))$ at point $(0.3H, 0.15H, -0.012H)$, circles: $T(\text{Ma}_3) - T(\text{Ma}_1)$ at point $(0.3H; 0.15H; -0.012H)$, dashed: difference between these two curves at the same point as functions of time

mean gas temperature and 3% in the droplet mean temperature. Moreover, we observe a close agreement between the results of the two codes in the droplet size PDF at a single time along with a good agreement in the Nusselt number history. This establishes the overall accuracy of the new low Mach number formulation.

It was shown that the time step in the low Mach number code can be chosen independently of Mach number. This was observed from numerical experiments at different low Mach numbers, which confirms the analysis of the dependence of the governing equations on Mach number. As a result, the flow at the realistic Mach number of $\text{Ma} = 0.005$ for the current flow conditions can be simulated approximately 250 times faster with the new solver. This gain in time will be used in future work to examine different initial conditions which give rise to processes where compressibility effects become more important.

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Chapter 5

Heat transfer in droplet-laden turbulent channel flow with phase transition in the presence of a thin film of water

Abstract

We present results of a study of turbulent droplet-laden channel flow with phase transition in the presence of gravity in the wall-normal direction and a thin film of water at the bottom wall. We maintain the film thickness constant by draining water from the bottom wall to compensate for (a) the droplets that fall onto the film and (b) evaporation/condensation. We also maintain on average the total mass of water in the channel by inserting new droplets at the top wall to compensate for the water that has been drained from the bottom wall. We analyze the behavior of the statistically averaged gas and droplet quantities focusing on the heat exchange between the two phases. We increase (a) the initial droplet diameter keeping the same initial droplet volume fraction and (b) the initial number of droplets in the channel keeping their diameter the same. In both parameter studies we find that droplets grow less than in the reference case. In case (a) this is explained by the larger velocity with which they travel to the bottom wall and in case (b) by the lower rate of condensation of vapor due to the presence of neighboring droplets.

5.1 Introduction

In the field of multiphase systems droplet-laden channel flow presents a challenging topic not only because of how turbulent flow influences the mass and heat transfer properties of droplets but also how, in turn, droplets modulate the flow. In particular, the two-way coupling influences the heat transfer which is relevant both in nature and in industrial applications. Important examples are cloud formation and particle dispersion in atmosphere and oceans along with combustion in engines and heat transfer in power stations (Barigou et al. 1998). Several studies dedicated to multiphase flows with a large number of dispersed droplets have been conducted. The first investigation was done by Mashayek (1998). He applied an Euler-Lagrange approach to describe two phases which were coupled by transfer of momentum, mass and energy. Later, a study of the mixing layer with embedded evaporating droplets was conducted by Miller and Bellan (1998). The presence of evaporating droplets in a turbulent planar jet was investigated by Masi et al. (2010). We focus on a new setting of a wall-bounded turbulent flow in which droplets not only evaporate, like in the studies cited above, but also

condensational growth due to the interaction with the vapor phase is dynamically important. We focus on the enhancement of the heat transfer between the channel walls. The motivation for this setting comes from the previous work of Kuerten et al. (2011), where it was shown that the presence of particles increases the Nusselt number by more than a factor of two. In this study we add several new features into the system among which phase transition one.

In this contribution we generalize earlier work by Bukhvostova et al. (2014a), Russo et al. (2014) and Bukhvostova et al. (2014b) and introduce gravity in the wall-normal direction which acts both on the flow and the droplets. Gravity leads to a mean motion of droplets towards the bottom wall where they accumulate and form a film of water. Initially we introduce a thin film of water at the bottom wall and account for droplets which fall into the film by adding new droplets at the top wall. In this paper we keep the film height constant by draining water from the film at the bottom wall and keep the surface of the film stationary.

First, we investigate the reference case for the flow conditions considered in Bukhvostova et al. (2014a) using 1 million droplets are initially distributed in the channel. We consider statistically averaged heat and mass transfer properties of the droplets and gas, obtained by averaging over all droplets present in the channel and over the periodic directions, respectively. To illustrate the included mechanisms better we also follow the trajectory of a single droplet, inserted at the top wall, and examine its motion and evolving properties. In real applications of systems with a large number of dispersed droplets, important parameters are the droplet size and the number of droplets. This motivates us to perform two additional sets of simulations. In the first we increase the initial droplet diameter keeping their initial volume fraction constant. In the second set of simulations, we increase the number of droplets up to 2 million keeping their initial diameter the same as in the reference case. We report and analyze differences in the results confronting them with the results of the reference case.

The computational setting is similar to a simple heat exchange widely used in industry (Abdul Karim et al. 2012). The better understanding of heat transfer enhancement for liquids and gases made it possible to incorporate different types of heat exchangers into gas turbines to improve their efficiency (McDonald et al. 2010). In our situation the heat exchange between the channel walls at given temperature difference between the walls is an important property to study.

The structure of the paper is as follows. In Section 2 the mathematical model for the two phases and for the film is given along with the details on the numerical method. In Section 3 we describe the initial conditions of the simulations. In Section 4 the results of the reference case and of the two sets of simulations are presented. Finally, we collect concluding remarks in Section 5.

5.2 Models and methods

This section is divided into four subsections. The first subsection is dedicated to the mathematical model for the gas and droplets which is identical to the model which was adopted in Bukhvostova et al. (2014a). In the second subsection we describe the model for the film of water. The third subsection is dedicated to the spatial discretization which is used in this study and finally, in the fourth subsection we give details on the time integration.

5.2.1 Mathematical model for the carrier and dispersed phases

We consider a water-air system in a channel, bounded by two parallel horizontal plates. In particular, a two-phase system, consisting of a carrier phase of dry air and water vapor and a dispersed phase of liquid water droplets next to a continuous water film will be investigated. The mixture of air and water vapor will be referred to as the carrier gas or gas and the liquid droplets as the dispersed phase. We use an Eulerian approach for the gas and track every droplet individually in a Lagrangian manner. In addition, we treat the carrier gas as compressible. In Figure 5.1 a sketch of the flow domain is presented. The domain has a size of $x_l = 4\pi H$ in the streamwise direction, which is denoted by x , and $z_l = 2\pi H$ in the spanwise direction, z , where H is half the channel height. In addition, y is the coordinate in the wall-normal direction. The top wall of the channel is located at $y = H$ and the bottom wall at $y = -H$. Studies done by Kim et al. (1987) motivate us to use periodic boundary conditions in the streamwise and spanwise directions. A thin film of water of a fixed thickness h is maintained at the bottom wall, such that $h \ll H$. The temperatures at the top and bottom walls of the channel are denoted by T_t and T_b , respectively, and kept fixed such that $T_t < T_b$. In addition, no-slip conditions are applied to the carrier phase at the upper wall and at the film surface. In this study we consider a simplified problem where the film surface does not move and is kept perfectly flat.

We consider the carrier phase to be a Newtonian fluid, whose behavior is described by the continuity equation, Navier-Stokes equation, energy conservation equation and vapor mass conservation equation. Droplets are described in a Lagrangian manner by a set of ordinary differential equations for the position, mass, velocity and temperature of each droplet. All details of the model can be found in Bukhvostova et al. (2014a).

An important new feature added in this study, is the presence of gravity. This leads to additional terms in the equations, which will be described next. First of all, the gravitational force will appear in the wall-normal momentum equations for the carrier gas and the droplets. We use the following model for the carrier phase (Bukhvostova et al. 2014a, Miller and Bellan 1998):

$$\partial_t \rho + \partial_j (\rho u_j) = Q_m \quad (5.1)$$

$$\partial_t (\rho u_i) + \partial_j (\rho u_i u_j) = -\partial_j \pi_{ij} + F_i + Q_{mom,i} + g_i \rho \quad (5.2)$$

$$\partial_t e_t + \partial_j (\rho u_j e_t) = -\partial_j q_j - \partial_j (u_i \pi_{ij}) + Q_e \quad (5.3)$$

$$\partial_t (\rho Y_v) + \partial_j (\rho u_j Y_v) = -\partial_j J_{v,j} + Q_m \quad (5.4)$$

where $Q_m, Q_{mom,i}, Q_e$ are sink/source terms expressing the two-way coupling between the carrier and droplet phases. These will be discussed later. In addition, (ρ, u_j, e_t, Y_v) are the carrier phase mass density, components of the velocity, total energy density and vapor mass fraction, respectively. Moreover, π_{ij} defines pressure and viscous contributions to the momentum flux; we use Sutherland's law to compute the dynamic viscosity. Among the components of the gravity vector $\mathbf{g}$ only the vertical component g_2 is not equal to zero. The term F_i is an external force density which is obtained from the conservation of total streamwise momentum in time. In addition, q_j denotes the components of the heat flux vector, which consists of heat transport by conduction and by diffusion and the vector J_v defines the diffusive mass flux of water vapor and the flux caused by the pressure gradient. The pressure and temperature of the carrier phase are denoted by p and T . The vapor mass fraction, p and T are connected by the

ideal gas law for an air-water vapor mixture given by Miller and Bellan (1998) :

$$p = \rho T R_{air}(1 - Y_v) + \rho T R_{water} Y_v \quad (5.5)$$

where R_{air} and R_{water} stand for the specific gas constants for air and water vapor, respectively. They are equal to the universal gas constant, divided by the corresponding molar mass. The presence of gravity leads to a potential energy density contribution to the total energy density of the gas, which is equal to:

$$e_{pot} = \rho g z \quad (5.6)$$

The total energy density e_t equals:

$$e_t = e_{kin} + e_{int} + e_{pot} \quad (5.7)$$

and two other contributions e_{kin} and e_{int} are specified in Bukhvostova et al. (2014a).

Two-way coupling between the two phases is implemented via momentum, energy and mass source terms in the governing equations of the carrier phase by requiring conservation of mass, momentum, energy and vapor mass (Bukhvostova et al. 2014a). The thin film, located at the warmer bottom wall, can contribute to evaporation and water vapor can also condense on its surface. We will give the mathematical formulations for these mechanisms when discussing the model for the film.

Fig. 5.1: Sketch of channel geometry, bounded by two horizontal planes, with water droplets and film of fixed height h . The size of the computational domain in the periodic stream- and spanwise directions is equal to $4\pi H$ and $2\pi H$, respectively, where H is half the channel height. The temperature at the bottom and top wall is kept constant, equal to T_b and T_t , respectively.

5.2.2 Simplified model for the film

Formally the thin film at the bottom channel wall requires the solution of a partial differential equation for its temperature as a function of time and the spatial coordinates. However, in this study we approximate the temperature in the film by a second-order polynomial in the wall-normal coordinate, closely following Russo et al. (2014b), as will be discussed in detail further in this chapter. Along with the film temperature T_f we also consider the film energy per unit area E_s since for the carrier gas we solve the system of equations for the conservative variables (5.1)-(5.4) and for the film we also choose a conservative variable. This choice will also simplify the requirement of continuity of the energy flux at the film interface which we will discuss later in this subsection.

There are three origins of change in the film energy: evaporation of water from the film surface or condensation of vapor onto the film surface, the conductive heat transfer from/to the gas and the droplets merging with the film because of gravity. All three mechanisms are discussed in this subsection.

The film is assumed to be sufficiently thin so that derivatives of its temperature parallel to the film are so small compared to derivatives in the wall-normal direction that they can be neglected. At the same time when droplets merge with the film, they bring locally diffusive and convective fluxes in the periodic directions parallel to the walls, which can not be neglected. The film is assumed not to move, consequently, the convective flux is not taken into account. These assumptions and simplifications permit to write the change in the film energy per unit area as:

$$\frac{\partial E_s}{\partial t}(x, z) = q_2 - q_1 + s_2 - s_1 \quad (5.8)$$

where q_1 and q_2 represent the fluxes in the wall-normal direction at the bottom wall $y = -H$ and at the film interface $y = -H + h$, respectively. Source terms s_1 and s_2 refer to changes in energy at the bottom wall and at the film interface, respectively, which will be specified below. The energy flux at the bottom wall is given by thermal conduction:

$$q_1 = k_w \left. \frac{\partial T_f}{\partial y} \right|_{y=-H} \quad (5.9)$$

where k_w is the thermal conductivity of water and T_f denotes the film temperature. The energy flux at the interface contains the conductive transport of energy between the gas above the film and the film surface:

$$q_2 = k_g \left. \frac{\partial T_g}{\partial y} \right|_{y=-H+h} \quad (5.10)$$

where k_g and T_g are the thermal conductivity and the temperature of the gas, respectively. The thickness of the film can change because of two reasons: (1) the film evaporates or water vapor condenses on the film and (2) droplets fall and merge with the film because of gravity. These two contributions compose the source term s_2 at the interface of the film with the carrier gas. We assume that at the liquid/carrier gas interface a mass $\dot{m}_v$ of water evaporates or condenses per unit time and per unit area of the film. If $\dot{m}_v$ has a negative sign, then evaporation from the film surface occurs; if it is positive, then water vapor condenses on its surface. This quantity $\dot{m}_v$ is modeled in a similar way as the evaporation from a spherical

droplet (Bukhvostova et al. 2014a):

$$\dot{m}_v = \frac{D\rho_g}{\delta} (Y_{v,\delta} - Y_{v,s}) \quad (5.11)$$

where D is the diffusion coefficient of water vapor in air and ρ_g is the carrier gas density. Moreover, $Y_{v,\delta}$ and $Y_{v,s}$ denote the vapor mass fraction at a small distance δ from the film surface in the carrier gas, and at the film surface, respectively. $Y_{v,s}$ is found from the saturation condition at the film interface computed using Antoine's law (Antoine 1888) while we choose to compute $Y_{v,\delta}$ at the first cell-center in the carrier gas for convenience. Consequently, δ is equal to the distance between the first cell center and the film interface. We model the film evaporation or the condensation on its surface of the water vapor in this way because this is consistent with the expression for the flux $J_{v,j}$ in (5.4). The combination of (5.11) and the expression for the vapor flux $J_{v,j}$ in (5.4) results in a constant vapor mass density in time in case the vapor mass fraction is a linear function of the wall-normal coordinate between the film interface and the second grid cell.

In order to maintain a constant film thickness we extract or add water at the bottom of the film. This defines the source term s_1 in (5.8). We compute the net amount of water $\dot{m}$ which enters/leaves the film in the form of water droplets $\dot{m}_d$ and water vapor $\dot{m}_v$ through the film interface per unit area per unit time:

$$\dot{m} = \dot{m}_d + \dot{m}_v \quad (5.12)$$

Consequently, the energy source at the bottom of the film is:

$$s_1 = \dot{m} c_w T_b \quad (5.13)$$

where c_w is the specific heat of water. In this way we maintain a constant film thickness h . The criterion for merging of a droplet with the film is that the distance between the droplet center of mass and the film surface is smaller than its radius.

In order to maintain on average a constant mass of water in the channel we distribute new droplets from the top wall according to the following procedure. The diameter of the inserted droplets is taken equal to the initial diameter d_0 and the corresponding mass of one droplet is denoted by m_0 . Each stage of a time step we determine the mass of droplets that should be inserted to keep the total mass of water in the system constant. This mass will in general not correspond to an integer number of droplets of mass m_0 . Therefore, we insert the nearest integer just below this value and keep the remainder for the next stage. In this way, on average the total mass of water is kept constant. The droplets are inserted at random locations at the top wall at the temperature of the top wall T_t . The stream- and spanwise velocity components of these droplets are equal to zero and the wall-normal component is equal to the terminal velocity which is found in the following way. Two forces are acting on a droplet: drag force and gravitational force. For the drag force we use the Schiller-Naumann correlation (Schiller and Naumann 1933). The droplet terminal velocity is defined from the condition that two forces balance, so that the acceleration of the droplet is equal to zero. This results in the following expression for the absolute value of the terminal velocity:

$$v_T = \frac{\tau_d g}{1 + 0.15 \text{Re}_d^{0.687}} \quad (5.14)$$

where τ_d is the droplet relaxation time, g denotes the absolute value of the gravitational acceleration and Re_d is the Reynolds number based on the droplet diameter and its velocity relative to the gas velocity at the droplet position which is taken to be zero up to a good approximation since we insert droplets at the wall. Equation (5.14) is a nonlinear equation. We find v_T iteratively once by first setting $Re_d = 0$ and then each iteration calculating Re_d from the terminal velocity found in the previous step until this method converges.

In addition, we define the energy of the droplets which enter the film per unit area per unit time by $\dot{E}_d$. This is equal to the sum of kinetic, potential and internal energy of the droplets which merged with the film per unit area per unit time. In our simplified model we sum the energy of all droplets which merge with the film and distribute it uniformly over the total film. Since we do not take into consideration the local change of the film height caused by droplet merging with the film, the corresponding energy is not be added locally as well but averaged over the total film. Consequently, s_2 can be written as:

$$s_2 = \dot{m}_v h_w + \dot{E}_d \quad (5.15)$$

where h_w is the specific enthalpy of liquid water.

Since some terms in the proposed model contain the film temperature, for instance, the conduction term (5.9), we also need the film temperature T_f as a function of the wall-normal coordinate. The relation between the film energy and the film temperature is:

$$c_w \rho_w \int_{-H}^{-H+h} T_f(x, y, z) dy = E_s(x, z) \quad (5.16)$$

where ρ_w denotes the mass density of water.

Since the film height is very small compared to the height of the channel, instead of discretizing the film, we approximate the film temperature by a second-order polynomial in the wall-normal coordinate, closely following Russo et al. (2014b).

$$T_f(x, z, y, t) = A_0(x, z, t) + A_1(x, z, t) \frac{y+H}{h} + A_2(x, z, t) \frac{(y+H)^2}{h^2} \quad (5.17)$$

The coefficients in (5.17) are recovered from the boundary conditions on the bottom wall and on the film surface. The following conditions should be satisfied. The first condition is the prescribed temperature at the bottom wall, T_b :

$$T_f \Big|_{y=-H} = T_b \quad (5.18)$$

The second boundary condition is the continuity of the heat flux at the interface. It is given by:

$$-k_w \frac{\partial T_f}{\partial y} \Big|_{y=-H+h} + h_v \dot{m}_v \Big|_{y=-H+h} = -k_g \frac{\partial T_g}{\partial y} \Big|_{y=-H+h} + h_w \dot{m}_v \Big|_{y=-H+h} \quad (5.19)$$

where h_v is the enthalpy of water vapor. The left-hand side of (5.19) is the flux into the gas at the film interface which has two contributions: the conductive term in the film and the term from evaporated/condensed vapor from/on the film surface. In a similar way we write the flux into the film which also reflects two mechanisms: conductive transport in the gas and the contribution from evaporation or condensation.

The final condition is the expression for the film energy per unit area E_s in terms of the film temperature, (5.16). From the three described conditions the three unknown coefficients in the polynomial representation of the film temperature (5.17) can be determined.

5.2.3 Spatial discretization

The spatial discretization of the equations in the gas is based on a finite volume method which follows the method in Bukhvostova et al. (2014a). The geometry is divided into rectangular cells. A uniform grid is used in the two periodic directions. In the wall-normal direction a non-uniform grid is applied which is finer near the walls in order to resolve the boundary layers. We apply the same non-uniform grid in the wall-normal direction as in Bukhvostova et al. (2014a) but the height of the first cell is smaller since it starts from the film interface $y = -H + h$. The film thickness is taken equal to $1/3$ of the height of the first cell. The variables are stored in the centers of the cells. We use 128 cells in each direction. This choice for the resolution is motivated in detail in Marchioli et al. (2008) where simulation results obtained with various numerical methods are compared. In that paper, simulations of a particle-laden turbulent channel flow at $Re_\tau = 150$ using second-order central differences, similar to our method, on the same grid as used here were reported. The results of this simulation showed a difference on the order of 1% in the mean velocity profile and on the order of 2% in the RMS of fluctuating quantities with other studies based on, e.g., pseudo-spectral methods. Moreover, in Bukhvostova et al. (2014b) we performed a simulation on a finer grid with 192 points in each direction and found that this grid refinement leads to differences on the order of less than 1% between the averaged results.

5.2.4 Time integration

In Bukhvostova et al. (2014a) explicit four-stage low-storage Runge-Kutta time-stepping was adopted. This time-stepping method is a second-order low-storage algorithm, in which the solution needs to be stored at the previous time and at the current stage only. In the current problem droplets can enter the film at any stage of a time step. This motivates us to apply another time integration procedure proposed by Spalart et al. (1991). The main differences between these two Runge-Kutta methods are that Spalart's method consists of three stages and that in order to compute the value of a variable at the new stage the values at up to two previous stages are required and not at the old time. For convenience we denote the algorithm used in Bukhvostova et al. (2014a) by RK4 and we will refer to the algorithm proposed by Spalart and used here as RK3.

RK3 method is a hybrid implicit-explicit time iteration method. For the nonlinear terms each stage is analogous to forward Euler or second-order Adams-Bashforth but with different coefficients while for the linear part the method is similar to the Crank-Nicolson scheme but again with different coefficients. The coefficients are derived from the condition of highest possible order of the algorithm and can be found in Spalart et al. (1991). In the present work we only use the explicit part of the algorithm and write the system of governing equations for

the carrier gas (5.1)-(5.4) in the following way:

$$\frac{\partial \mathbf{w}}{\partial t} = N(\mathbf{w}) \quad (5.20)$$

where $\mathbf{w}$ stands for the vector of variables which are mass density, momentum, total energy density and water vapor mass density: $\mathbf{w} = [\rho, \rho \mathbf{u}, e_{tot}, \rho Y_v]$. The right-hand side of (5.20) is the sum of convective and viscous terms of the governing equations for the carrier phase. In a similar way we also apply only the explicit part of RK3 to the system of ordinary differential equations for the droplets. The treatment of the right-hand sides of the systems of equations for the gas and droplets system of equations as nonlinear terms guarantees the third-order accuracy of the scheme.

The disadvantage of RK3 is a slightly more severe restriction on the time step. We show this performing a stability analysis for the system of equation (5.1)-(5.4) and two time integration schemes in the same way as done by Müller and Rizzi (1987) for an explicit algorithm for compressible, viscous flow. The stability analysis consists of two parts. First, the equations are linearized and discretized in space. This leads to a large system of coupled, linear ordinary differential equations. Fourier analysis results in a diagonal system of equations of the form:

$$\frac{d\mathbf{v}}{dt} = \Lambda \mathbf{v} \quad (5.21)$$

where $\mathbf{v}$ represents the vector of amplitudes of the Fourier modes and Λ is a diagonal matrix which contains the complex eigenvalues, λ_i . Second, the regions in which $\lambda_i \Delta t$ is stable for the specific Runge-Kutta schemes are determined.

Following Müller and Rizzi (1987) for our systems of equations, we find that the diffusive terms in the equations lead to:

$$\frac{-4}{\text{Re}_b \text{Sc} \Delta x^2} < \text{Re}(\lambda_i) < 0 \quad (5.22)$$

At the same time the convective terms lead to:

$$|\text{Im}(\lambda_i)| < \frac{u}{\text{Ma} \Delta x} \quad (5.23)$$

which is a more severe restriction on the time step than (5.22) and defines the limiting value for the time step.

Figure 5.2 shows the regions in which $\lambda_i \Delta t$ should be to obtain stability for both algorithms. From this figure we find that RK4 and RK3 are stable for $\Delta t \leq \text{CFL} \times \text{Ma} \frac{\Delta x}{u}$ with $\text{CFL} = 2$ and $\text{CFL} = 1$, respectively. From numerical tests we also found that the optimal time step in RK3 is twice smaller than in RK4. With this time step we are still in the regime of affordable computing times, also because the CPU time of one time step of RK3 is smaller than that of RK4. This results in approximately the same computing time of the full simulation for both integration methods.

One stage of a time step is executed in the following order. First, we find the properties of the droplets at the new stage, then we renew the properties of the carrier gas and finally, we solve the system of equations for the film. This order is motivated by the occurrence of the gas temperature at the new stage in equation (5.19) for the film. In order to calculate the gas temperature at the new stage the two-way coupling terms, which are directly connected to the

system of ordinary differential equations for the droplets (Bukhvostova et al. 2014a), need to be known.

In the next section we will give the details on the initial conditions for the simulations along with the validation of the model and results of the simulation cases.

Fig. 5.2: The outer bound of the stability region for solid: RK4 dashed: RK3. The figure shows the region in which the amplification factor of the scheme is smaller than 1.

5.3 Initial conditions and simulation cases

In this subsection we specify initial conditions for the carrier gas, film and droplets. Then, we introduce two sets of simulations which we perform in this study.

We start the simulations from turbulent velocity, density and temperature fields obtained from a simulation without droplets and with adiabatic boundary conditions at the walls (Bukhvostova et al. 2014a). This simulation was performed until a statistically steady state was reached. In the present study we keep the wall temperatures constant. We keep the temperature difference between the walls equal to 3K choosing $T_b = 293.15\text{K}$ and $T_t = 290.15\text{K}$. This temperature difference is the same as in the steady state in the reference case in Bukhvostova et al. (2014a) where we applied a constant heat flux through the walls. The reference case was initialized with ‘mild’ conditions, such as room temperature, atmospheric pressure and saturated vapor pressure. In this paper we make the setting as close as possible to a possible experiment, using fixed wall temperatures.

The reference scales of the system define the non-dimensional parameters, such as the

Reynolds number based on the bulk velocity Re_b , the Mach number Ma , the Prandtl number Pr and the Schmidt number Sc , along with the thermodynamic parameters of the simulations. We choose the same reference scales as in the reference case in Bukhvostova et al. (2014a). The reference temperature and mass density are equal to the mean initial temperature and mass density. Specifically, the reference temperature is taken equal to room temperature, $T_{ref} = 293.15K$. The reference velocity is taken as the initial bulk velocity of the carrier gas. The reference length is chosen as half the channel height. From the initial pressure, which is taken as the atmospheric pressure, and the initial relative humidity of 100% everywhere in the channel we find the initial mass density of the carrier gas and the initial vapor mass fraction. The thermodynamic values of the system along with the non-dimensional parameters are shown in Table 5.1.

Initially, we take the film temperature uniform and equal everywhere to T_b . The gas temperature above the film surface is slightly larger than 293.15K and this leads to initial condensation of water vapor on the film surface.

We randomly distribute droplets over the volume of the channel. We define a reference case in which the initial number of droplets is equal to 1,000,000 and the initial diameter d_0 is 3.09×10^{-3} in non-dimensional units. We perform two sets of simulations which are described in Table 5.2. In the first set we vary the initial number of droplets keeping their initial volume fraction equal to that used in the reference case. As a consequence, the initial droplet diameter is different, Table 5.2. In the second set of simulations we increase the initial number of droplets to 2,000,000 keeping their initial diameter the same. The droplet volume fractions in the performed simulations correspond to the two-way coupling regime according to the classification proposed by Elghobashi (1994).

In this paper we use the point-particle approach. This is allowed if the droplet diameter is sufficiently smaller than the Kolmogorov length (Marchioli et al. 2006). In the channel flow the Kolmogorov length varies along the wall-normal direction from a minimum value of 1.6 near the wall to a maximum value of 3.6 in wall units at the centerline (Marchioli et al. 2008). In this paper we consider three different initial droplet diameters. For the largest value of the diameter the maximum ratio of the droplet diameter, which in wall units equals 0.8, and the Kolmogorov scale is approximately 0.48. This we adopt as sufficient motivation for using the point-particle approach.

K , (W/m · K)	μ , (kg/m · s)	D , (m ² /s)	Re_b	Pr	Ma	Sc
2.5519×10^{-2}	1.86766×10^{-5}	2.0917×10^{-5}	2333	0.7478	0.05	0.6283

Table 5.1: Thermodynamic and non-dimensional parameters of simulations

5.4 Results of the film simulations

In this section we will first discuss in detail the results of reference case 1M and then investigate the differences between the reference case and other test cases in the two series of simulations described in the previous section.

case	N^0 drop	d_0	V_0
1M	1million	3.09×10^{-3}	10^{-4}
M/2	1/2 million	3.89×10^{-3}	10^{-4}
M/4	1/4 million	4.91×10^{-3}	10^{-4}
V	2 million	3.09×10^{-3}	2×10^{-4}

Table 5.2: The test cases. N^0 drop, d_0 and V_0 denote the initial number of droplets, initial droplet diameter and their initial volume fraction.

In the analysis of the behavior of droplets and gas we focus on the evolution of mean quantities which are averaged over the periodic directions. The averaging is denoted by brackets, $\langle \cdot \rangle$. The averaging procedure is different for the carrier and dispersed phases. For the carrier gas we know the values at the cell centers and we can easily perform averaging over the stream- and spanwise directions. For the droplets we use the following technique. At each time we average all quantities of interest by averaging over all droplets which are located in a slab parallel to the walls around a certain wall-normal coordinate. We use 128 slabs in the wall-normal direction. The boundaries of these slabs correspond to the grid locations used in the wall-normal direction for the gas. This implies that the averaged carrier gas and droplet quantities are known at the same locations in wall-normal direction. All quantities are presented in dimensional units. In all figures where results at different times are shown, the arrow denotes the direction of time.

The structure of this section is as follows. It consists of three subsections dedicated to the analysis of the reference case, to the first and to the second set of simulations, respectively. The first subsection is divided into two parts. The first one is dedicated to the kinematic properties of the system and the second to the thermal characteristics.

5.4.1 Results of reference case 1M

5.4.1.1 Velocity properties of droplets

We examine the mean wall-normal component of the droplet velocity at different times as a function of the wall-normal coordinate in Figure 5.3a. The terminal velocity in case 1M is equal to 0.103 m/s, equation (5.14). In Figure 5.3a we observe that the mean wall-normal droplet velocity deviates from the terminal velocity by up to 25%. The theoretical value of the terminal velocity is derived under the assumption of laminar flow. Apparently, turbulence results in an increase of the wall-normal velocity, especially away from the walls, where the fluctuations in the wall-normal gas velocity are highest. Close to both walls the mean wall-normal droplet velocity is slightly smaller than the terminal velocity. The RMS of the wall-normal droplet velocity component, which is shown in Figure 5.3b, is of the same order of magnitude as its mean value. It is known that this leads to complex motion of bubbles in turbulent flow from Sene et al. (1994), Spelt and Biesheuvel (1997). Even though a different system was investigated in these papers - gas bubbles in a turbulent flow of water - we observe a similar behavior for droplets in a turbulent flow of gas.

Based on the results shown in Figure 5.3a, we made an estimate of the rate at which droplets

are inserted from the top wall. We first calculate how long it takes for one droplet on average to travel through the channel:

$$\langle t_{tr} \rangle = \int_{y=-H}^{y=H} \frac{dy}{\langle u_y \rangle} \quad (5.24)$$

where $\langle t_{tr} \rangle$ denotes the average travel time for one droplet and $\langle u_y \rangle$ is the mean wall-normal velocity of droplets shown in Figure 5.3a. Knowing $\langle t_{tr} \rangle$, we also know after how much time we should insert a new droplet from the top wall to keep the total water mass conserved. In other words, the frequency with which we have to replace one droplet is $\frac{1}{\langle t_{tr} \rangle}$. Multiplying this by the total number of droplets in the channel, we obtain the estimate for the rate. In order to verify this estimate we performed a simulation during a time interval $[0; T_s]$ with T_s equal to 2 s and we determined N_{ins} , the number of droplets inserted from the top wall during this time interval, consistent with the condition that the average water content in the system is kept virtually the same. We verify that:

$$\frac{N_{ins}}{T_s} \simeq \frac{\langle N_{total} \rangle_{T_s}}{\langle t_{tr} \rangle} \quad (5.25)$$

where $\langle N_{total} \rangle_{T_s}$ is the mean number of droplets present in the channel during the time T_s . The left-hand side of (5.25) equals 3065432 droplets per second, whereas the right-hand side of (5.25) equals 2890193 droplets per second. The difference between these two values is on the order of 6%.

Fig. 5.3: (a) Mean wall-normal droplet velocity (b) RMS of wall-normal droplet velocity as functions of the wall-normal coordinate at different times. Dashed line: initially, square-marked: 0.5 s, circle-marked: 1.0 s, solid: 3 s

5.4.1.2 Heat and mass transfer results

In Figure 5.4 we show the development in time of the mean gas temperature as a function of the wall-normal coordinate. We start from a statistically steady turbulent solution with adiabatic boundary conditions and at $t = 0$ suddenly impose fixed temperatures at both walls, in which the temperature at the top wall is lower than at the bottom wall. This causes the development and propagation of a thermal front from the colder top wall of the channel to the warmer bottom wall. We consider separately the history of the mean gas temperature near the top wall and in the center of the channel, Figure 5.5. This figure shows that indeed the temperature near the top wall starts decreasing almost immediately, while it takes some time before the temperature in the center of the channel decreases. The mean gas temperature near the top wall initially decreases significantly because of the imposed lower temperature at the top wall, Figure 5.5a, which leads to supersaturation of the gas. This can be seen in Figure 5.6, which shows the history of the mean relative humidity near the top wall. We observe a jump at $t = 0$ starting from the initial saturation condition up to a value of around 120%.

We also considered the history of the mean gas temperature at the first cell center, Figure 5.7. We see that it also takes some time before the thermal front reaches the bottom wall of the channel. We examine the evaporation and condensation behavior of the film interface by considering the term $\frac{dm_v}{dt}$ averaged over the periodic directions as a function of time in Figure 5.8a. We observe the evaporation of the film only during the initial stages of the simulation. This is explained by the initial condition, in which the temperature of the film is slightly higher than that in the first cell above the film. Later in time water vapor condenses on the film surface. The mean relative humidity history at the first cell center is shown in Figure 5.8b. The oversaturation is explained by the decrease of the mean temperature shown in Figure 5.7, and the approximately constant amount of water vapor in this region.

We start the analysis of the droplets by considering the mean rate of droplet mass change, $\frac{dm_d}{dt}$, in Figure 5.9. We observe growth of droplets everywhere in the channel as a result of a net condensation of vapor from the gas onto the droplets. In order to analyze better this behavior we focus the analysis on the region near the colder top wall considering the algebraic expression for $\frac{dm_d}{dt}$ which is:

$$\frac{dm_d}{dt} = -\frac{m_d \text{Sh}}{3 \tau_d \text{Sc}} \ln \left(\frac{1 - Y_{v,\delta,d}}{1 - Y_{v,s,d}} \right) \quad (5.26)$$

where m_d and τ_d are the droplet mass and relaxation time, respectively. Moreover, Sh is the Sherwood number for which we use an empirical correlation; further details can be found in Bukhvostova et al. (2014a). The driving quantity in (5.26) is the difference $Y_{v,\delta,d} - Y_{v,s,d}$ where $Y_{v,\delta,d}$ and $Y_{v,s,d}$ are the vapor mass fractions at a distance δ from the surface of the droplet and on the surface of the droplet, respectively. For small values of the vapor mass fractions, the rate of mass change of a droplet is approximately proportional to $Y_{v,\delta,d} - Y_{v,s,d}$ which can be also written in the following way using the definition of relative humidity (Incropera et al. 2007):

$$Y_{v,\delta,d} - Y_{v,s,d} = \text{RH}(\mathbf{x}_d, t) \frac{p_{\text{sat}}(T(\mathbf{x}_d), t)}{T(\mathbf{x}_d, t)} - \frac{p_{\text{sat}}(T_d)}{T_d} \quad (5.27)$$

Fig. 5.4: Mean gas temperature as a function of the wall-normal coordinate plotted every 0.2 s in the interval $[0s, 3s]$. The dashed line corresponds to $t = 0$.

Fig. 5.5: History of mean gas temperature (a) near the top wall (b) in the center of the channel

Fig. 5.6: Mean relative humidity, averaged over the periodic directions, at one point near the top wall as a function of time. The insert shows the behavior at early times, markers show when the data are recorded.

Fig. 5.7: History of mean gas temperature at the first cell center in the carrier gas from the film interface

Fig. 5.8: History of mean of (a) term $\frac{dm_v}{dt}$ (b) relative humidity at the first cell center in the carrier gas from the film interface

where $RH(\mathbf{x}_d, t)$ and $T(\mathbf{x}_d, t)$ are the relative humidity and gas temperature at the droplet location $\mathbf{x}_d$ and p_{sat} and T_d denote the saturation pressure and droplet temperature, respectively. In our simulation droplets grow because of a combination of: the larger gas temperature at the droplet location compared to the droplet temperature, Figure 5.10a, and the high value of the relative humidity at the droplet location. The saturation pressure p_{sat} is calculated using Antoine's relation (Antoine 1888):

$$p_{sat} = 10^5 \exp \left(A - \frac{B}{C + T_d} \right) \quad \text{in Pa} \quad (5.28)$$

where $A = 11.6834$, $B = 4089.59$ K and $C = 500.02$ K. Consequently, the function $\frac{p_{sat}(T)}{T}$ is an increasing function of temperature. The positive value of the difference between $T(\mathbf{x}_d, t)$ and T_d on its own already results in positive values of the difference $\frac{p_{sat}(T(\mathbf{x}_d, t))}{T(\mathbf{x}_d, t)} - \frac{p_{sat}(T_d)}{T_d}$ near the top wall as shown by the insert in Figure 5.10b. The fact that the gas temperature is higher than the droplet temperature is explained by the quite rapid movement of cold droplets, inserted from the top wall, towards the bottom wall during which they do not have sufficient time to adapt to the temperature of the surrounding carrier gas. The vapor condensation on the droplet surface is augmented by the high relative humidity near the top wall, as the dashed-dotted line in Figure 5.10b shows.

We performed the same analysis of the individual terms on the right-hand side of (5.27) near the film interface. Figure 5.11 shows that initially droplets evaporate in this region since their temperature is larger than the temperature of the surrounding gas and the value of the relative humidity is not large enough to compensate this temperature difference. Further in time water vapor condenses on their surface since colder droplets from the top wall reach the region near the bottom wall. Moreover, the larger value of the relative humidity also contributes to the growth of droplets.

The mechanism behind droplet growth can be illustrated better by following the trajectory of

one droplet which is inserted at the top wall and monitoring its properties in time. We first consider the wall-normal coordinate and velocity component of the droplet in Figure 5.12. The wall-normal velocity component fluctuates considerably in time, sometimes even becoming positive. This could be expected from Figure 5.3b, which shows that the RMS of the wall-normal droplet velocity component is of the same order of magnitude as its mean value. There are also droplets which move with higher velocity towards the bottom wall. In addition, we consider this droplet's condensation rate as a function of time in Figure 5.13. We observe that the droplet grows during most of the time while falling towards the bottom wall. Second, we consider the history of the gas temperature at the droplet location and the droplet temperature in Figure 5.14a. We see that while the droplet is located near the top cold wall its temperature is smaller than the temperature of the surrounding gas; later in time the temperature difference decreases and eventually the two temperatures are almost equal and the difference is sometimes positive, sometimes negative. This behavior is analyzed in more detail by considering the temperature equation of a droplet. The droplet temperature changes because of two reasons: (1) condensation on the droplet surface and (2) temperature difference between the droplet and the surrounding gas:

$$\frac{dT_d}{dt} = \frac{\lambda_v \frac{dm_d}{dt}}{c_w m_d} + \frac{h_m A_d (T(\mathbf{x}_d, t) - T_d)}{c_w m_d} \quad (5.29)$$

where λ_v is the specific enthalpy of evaporation, h_m is the heat transfer coefficient and A_d denotes the surface area of the droplet. We show the history of the two separate terms on the right-hand side of (5.29) in Figure 5.14b. We observe that the latent heat contribution $\frac{\lambda_v \frac{dm_d}{dt}}{c_w m_d}$ is dominant during the initial droplet movement, until $t = 0.02$ s. Later in time the two terms on the right-hand side of (5.29) have the same order of magnitude and attain both positive and negative values. This implies that the droplet intensively grows until a characteristic time $t = 0.02$ s during which the heat exchange with the carrier gas mainly occurs through the latent heat contribution. After this adaptation time the rate of droplet growth becomes smaller, Figure 5.13, and the droplet temperature is closer to the temperature of the surrounding gas, Figure 5.14a.

As the final characteristic of the droplet behavior we consider the evolution of the mean droplet diameter normalized by the initial diameter as a function of the wall-normal coordinate in Figure 5.15. A noticeable feature is the presence of a hump in this profile which moves and eventually disappears. It appears because of the intensive initial condensation of water vapor onto the droplet surface which is the result of the two mechanisms discussed above: first, the positive difference between the gas temperature at the droplet location and the droplet temperature and second, the high relative humidity. Droplets fall towards the bottom wall under the action of gravity and the hump moves with them. The hump disappears in time since the mean droplet growth rate decreases later in time because of the decreasing over-saturation, as shown in Figure 5.6 and Figure 5.9.

5.4.2 Comparison of the results of the first set of simulations

In this subsection we discuss the results obtained from cases M/2 and M/4 and compare them with the results from case 1M. First, we compare the kinematic properties, then we analyze

Fig. 5.9: History of mean rate of mass change of a droplet as a function of the wall-normal coordinate, plotted every 0.7 s in the interval [0 s; 3 s]. The dashed line shows $t = 0$.

Fig. 5.10: (a) History of mean difference between gas temperature at droplet location and droplet temperature, plotted every 0.7 s in the interval [0 s; 3 s]; (b) History of $RH(\mathbf{x}_i) \frac{p_{sat}(T(\mathbf{x}_i))}{T(\mathbf{x}_i)}$ (dashed-dotted), $\frac{p_{sat}(T(\mathbf{x}_i))}{T(\mathbf{x}_i)}$ (dashed) and of $\frac{p_{sat}(T_d)}{T_d}$ (solid) at the first cell center from the top wall. The insert shows the initial stage of the simulation in detail.

Fig. 5.11: History of $RH(\mathbf{x}_i) \frac{p_{sat}(T(\mathbf{x}_i))}{T(\mathbf{x}_i)}$ (dashed-dotted), $\frac{p_{sat}(T(\mathbf{x}_i))}{T(\mathbf{x}_i)}$ (dashed) and of $\frac{p_{sat}(T_d)}{T_d}$ (solid) at the first cell center from the bottom wall. The insert shows the initial stage of the simulation in detail.

Fig. 5.12: (a) Wall-normal coordinate (b) Wall-normal velocity component of the inserted droplet as functions of time.

Fig. 5.13: Mass rate history of a single droplet. The dashed line indicates the rate at $t = 0$.

Fig. 5.14: (a) Droplet temperature (dashed) and gas temperature at droplet position (solid); (b) History of first (dashed) and second term (solid) on the right-hand side of (5.29).

Fig. 5.15: Mean droplet diameter as a function of the wall-normal coordinate plotted every 0.2 s in the interval [0 s, 3 s]. The dashed line indicates the result at $t = 0$.

the differences in the droplet properties and in the mean gas temperature.

We compare the mean wall-normal droplet velocity component, normalized by the terminal velocity for each case, as a function of the wall-normal coordinate at time $t = 3$ s which is chosen to illustrate the typical results in Figure 5.16a. We see that variations of the mean droplet wall-normal velocity from the terminal velocity grow from 1% in case M/4 up to 10% and 20% in cases M/2 and 1M, respectively. The initial Stokes number equals 10.8, 17.1 and 27.1 in case 1M, M/2 and M/4, respectively. Changes in Stokes number due to the growth of droplets during a simulation are very small. Figure 5.16a shows that larger droplets with larger Stokes number are less affected by the turbulent character of the flow. We also compare the ratio of the RMS of the wall-normal gas velocity and the terminal droplet velocity in Figure 5.16b, which is observed to be larger in case 1M than in cases M/2 and M/4. The closer this ratio is to 1, the more the motion of bubbles is affected by turbulence according to Sene et al. (1994), Spelt and Biesheuvel (1997). We observe here the same behavior for water droplets in a gas flow.

We also consider the mean droplet diameter, normalized by its initial value, as a function of the wall-normal coordinate at two different times, $t = 0.1$ s and $t = 0.3$ s in Figure 5.17 which were chosen to show the typical behavior at an early and intermediate time. At the earlier time of $t = 0.1$ s a hump is present in all cases. This hump is larger for case 1M than for M/2 and M/4 which is explained by the faster movement of droplets towards the bottom wall in case M/4. Consequently, the droplets do not have enough time to grow by vapor condensation as in case 1M. The plot at the later time, Figure 5.17b, illustrates that the hump travels faster and disappears faster in case of larger droplets, because of the larger wall-normal velocity.

The difference in wall-normal droplet velocity explains the mean difference between the gas temperature at the droplet location and the droplet temperature shown in Figure 5.18a. In all cases relatively colder droplets move towards the bottom wall through the carrier gas which

has a higher temperature and a relative humidity larger than 100%. The larger droplets in cases M/2 and M/4 have a higher wall-normal velocity. Therefore, their residence time in the gas is smaller, but through their larger surface area the rates of heat and mass transfer with the carrier gas are larger. Note that both heat and mass transfer result in a temperature increase of the droplets, the latter by the latent heat associated with condensation of vapor on the droplet surface, while the former by direct conduction from the relatively warmer surrounding to the colder droplets. The results indicate that the smaller residence time has the biggest effect: a larger droplet size leads to a larger temperature difference between carrier gas and droplets. We consider the mean gas temperature as a function of the wall-normal coordinate for the three cases at $t = 0.5$ s in Figure 5.18b. The decrease of the mean gas temperature for increasing initial droplet size can be explained in the following way. Figure 5.18a showed that the larger the droplet size, the larger the temperature difference between carrier gas and droplets. The total droplet surface area also plays a role in the heat exchange between the two phases. We verified for the typical time $t = 0.5$ s that even though the total droplet surface area is larger in case 1M than in cases M/2 and M/4, this effect is outweighed by the larger temperature difference between gas and droplet in cases M/2 and M/4 than in 1M. This can be understood from the following. The droplet volume fraction V is in a good approximation in all three cases is constant and proportional to the number of droplets N and the droplet radius R to the third power:

$$V \propto NR^3 \quad (5.30)$$

At the same time the total droplet surface area A is proportional to the number of droplets N and to the square of the droplet radius R :

$$A \propto R^2 N \propto \left(\frac{V}{N}\right)^{2/3} N \propto N^{1/3} \quad (5.31)$$

where the last step follows since V is constant. We observe in Figure 5.18a that the mean difference between the gas temperature at the droplet position and the droplet temperature decreases faster than $N^{-1/3}$ with increasing number of droplets. Therefore, we conclude that the rate of heat exchange between droplets and carrier gas is larger for the cases with larger droplets.

5.4.3 Comparison of the results of the second set of simulations

In this subsection we compare the results from cases 1M and V by analyzing the effect of doubling the number of droplets in the system and keeping their size constant. We compare the mean droplet diameter normalized by its initial value as a function of the wall-normal coordinate at two characteristic times, $t = 0.1$ s and $t = 1$ s in Figure 5.19. The figure shows that in case V droplets grow less and the difference in droplet size compared to case 1M between the results of the two cases becomes more pronounced at later times. To understand this trend we will first consider two limiting cases. For very dilute systems, the effects of two-way coupling between gas and droplets are negligible. This means that droplets are not affected by the presence of other droplets. In such a case a doubling of the number of droplets will not change the results for mean droplet diameter and temperature. On the other hand, in the

Fig. 5.16: (a) Mean wall-normal droplet velocity normalized by the terminal velocity; (b) ratio of RMS of gas wall-normal velocity and terminal velocity as functions of the wall-normal coordinate at $t = 3$ s. Solid: case 1M, dashed: case M/2, circle-marked: case M/4.

Fig. 5.17: Mean droplet diameter normalized with its initial value as a function of the wall-normal coordinate at different times. (a) 0.1 s (b) 0.3 s. Solid: case 1M, dashed: case M/2, circle-marked: case M/4.

hypothetical case that the volume fraction of droplets is very large, they will influence each other, not only in terms of their motion via two-way coupling but also in terms of the mass transfer with the carrier gas. Condensation of vapor on one droplet will decrease the relative humidity near a neighboring droplet and influence the condensation rate on that droplet. If in such a case the number of droplets is doubled, the same amount of vapor is available for condensation on twice as many droplets and the growth of the droplets will be less by a factor of two. The results show that we are not in one of these limiting cases. In case V the growth of the mean droplet size is less than in case 1M, but the reduction is much lower than a factor

Fig. 5.18: (a) Mean temperature difference between the gas at droplet location and droplets; (b) mean gas temperature as functions of the wall-normal coordinate at $t = 0.5$ s. Solid: case 1M, dashed: case M/2, circle-marked: case M/4.

of two. In order to illustrate this further, we focus on the region near the top wall and consider the history of the relative humidity in this region for cases V and 1M in Figure 5.20. We observe a smaller relative humidity in case V, indicating that more vapor condensed onto the available droplets, but the change in RH is not twice as large in case V as in case 1M when considering the total effect over a longer interval, e.g. 1 second. For sufficiently small times the difference in the change in relative humidity is equal to 1.7 and closer to a factor of two than at later times, as can be seen in the inset in this figure. This indicates that the initial mass transfer is not yet affected much by the competition for vapor.

We consider the mean gas temperature at two times in Figure 5.21 which is found to be lower in case V than in case 1M. The situation is similar to the one described for the difference between cases M/4 and 1M in the previous subsection. In case V droplets grow less, so that their temperature increases less by the latent heat associated with condensation. Therefore, the mean temperature difference between the gas at the droplet location and droplet is larger in case V than in the reference case. Recalling the analysis in Bukhvostova et al. (2014a), we know that the main contribution to the change in gas temperature is $-\sum_d h_m A_d (T(\mathbf{x}_d, t) - T_d) \delta(\mathbf{x} - \mathbf{x}_d)$ in the two-way coupling term, where the sum is taken over all droplets in the domain. Both the larger difference $(T(\mathbf{x}_d, t) - T_d)$ and the larger number of droplets result in a larger change in the gas temperature which is observed in Figure 5.21.

5.5 Conclusions and future work

In this work turbulent droplet-laden channel flow with phase transition was studied in the presence of gravity in the wall-normal direction. The gravitational force motivated us to investigate the following setting. In the initial state we introduce at the bottom wall of the

Fig. 5.19: Mean droplet diameter normalized with its initial value as a function of the wall-normal coordinate at different times. (a) 0.1 s (b) 1.0 s. Solid: case 1M, dashed: case V.

Fig. 5.20: Mean relative humidity averaged over the periodic directions at one point near the top wall as a function of time. Solid: case 1M, dashed: case V. Insert shows in detail the initial time of simulations.

Fig. 5.21: Mean gas temperature as a function of the wall-normal coordinate at different times: (a) 0.1 s (b) 1.0 s; solid: case 1M, dashed: case V.

channel a thin film of water with a thickness which is kept constant in time. In addition, the surface of the film is treated as stationary. Because of the direction of the gravitational force from the top to the bottom wall, droplets move to the bottom wall and merge with the film. In order to keep a constant film thickness, we drain water from the bottom wall. In order to have on average the same total mass of water in the channel we add droplets at the top wall. In addition, we impose a temperature difference of 3 K between the channel walls, keeping the top wall colder than the bottom wall. The mathematical models for the carrier and dispersed phases are identical to the models in Bukhvosova et al. (2014a) and we solve an additional equation for the film energy per unit area which is coupled to the equations of gas and droplets.

We investigated the heat and mass transfer characteristics of the two phases for different process conditions. First, we focused on a reference case of 1 million droplets, initially present in the channel investigating both averaged properties and following the trajectory of one single droplet which is inserted at the top wall. We observed the development and propagation of a thermal front from the top wall to the bottom wall. Droplets tend to grow by condensation of vapor on their surface. We investigated the reason for this behavior by analyzing the rate of droplet mass change and droplet temperature. There are two reasons for the droplet growth. First, since the droplets move from a colder to a warmer region and need time to adapt to the local gas temperature, their temperature is in general lower than the temperature of the surrounding gas. Second, the relative humidity is larger than 100% due to the decrease of the gas temperature by the condition imposed at the upper boundary.

We performed two sets of additional simulations. In the first we vary the initial droplet diameter keeping their initial volume fraction the same. We considered two cases with initially 1/2 million and 1/4 million droplets and compared the results of these simulations with the reference case. The main conclusion is that in cases of larger initial droplet size they tend to fall towards the bottom wall faster and consequently, have smaller residence time in the gas. This results in less heat exchange between carrier gas and droplets and hence, in a smaller growth rate and larger temperature difference between the gas and droplets for the case of

larger droplets.

In the second set of simulations we increased the initial number of droplets present in the channel by a factor of two. Confronting the results with the results of the reference case, we found that in the case of a larger number of droplets they grow less because of a lower rate of condensation due to the presence of neighboring droplets.

In future we plan to quantify the effective heat transfer between the channel walls for all investigated cases in terms of the Nusselt number. Moreover, a more sophisticated model for the film will be developed including the following characteristics: the motion of the film and the change of the film thickness in time and space caused by the interaction between the film and the turbulent character of the flow above it.

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Chapter 6

Conclusions and Outlook

In this chapter main conclusions of this thesis are presented along with recommendations for further studying of the problem. The conclusions are grouped according to the chapters of the thesis.

In Chapter 2 we compared two approaches to model turbulent droplet-laden channel flow with phase transitions: compressible and incompressible formulations. The incompressible formulation was adopted by Russo et al. (2014). We confronted their results with the results of the compressible formulation. We found that the mechanical properties such as velocity profiles show close agreement with the difference less than 1%. At the same time the thermal transfer properties such as the Nusselt number, and the mass transfer properties of the dispersed droplets show significant systematic differences also in the limit of low Mach numbers, for which it is a common practice to use the incompressible formulation. The difference on the order of 10% in the prediction for the Nusselt number gives an evidence of the sensitivity of the system to compressibility effects even for low values of the Mach number.

Apart from investigation of the agreement between the results of the two formulations in the limit of the Mach number, we also studied the effects of heat flux variations and increasing of the temperature level in the system. We increased the value of the heat flux to the walls of the channel by a factor of five in one case and set the mean temperature within the channel equal to 323.15K instead of 293.15K. In these two cases the differences between two formulations become more pronounced as it was expected. For the case of increased heat flux to the walls a difference in the mean droplet diameter near the walls on the order of 5% was observed, while for the case of a higher mean temperature we see a significant difference in the Nusselt number of about 15%, showing the relevance of the compressible formulation. The conclusion of this study is that for the 'mild' initial condition incompressible and compressible formulations show quantitative close agreement, however for the predictions of the mass and heat transfer properties the compressible formulation is essential.

Chapter 3 of this thesis is dedicated to the investigation of more critical initial conditions of lower value of initial relative humidity which causes stronger mass initial transfer associated with the tendency of the system to reach the saturation condition. The larger variations in the vapor mass density lead to larger variations in the total mass density of the carrier gas. We investigated the heat transfer in the channel in the terms of the Nusselt number and we found that the relative difference in it between the results of compressible and incompressible formulations is 1.5 times larger in the case of lower initial relative humidity than in the 'mild' reference case from Chapter 2. That gives an additional evidence that for an accurate

quantitative prediction for the heat transfer in the droplet-laden turbulent channel flow with phase transition the compressible formulation may be needed.

The studies described in the previous two chapters were conducted using the fully explicit time integration method in which the time step suffers the severe restriction from a CFL condition for low Mach numbers. In Chapter 4 we described the development and testing of a new time integration algorithm in which the time step can be chosen independently of Mach number. The new algorithm is an extension of the numerical algorithm proposed by Bell et al. (2004) to the considered multiphase problem. The fully explicit algorithm belongs to the family of density-based methods, while the new developed method is a pressure-based method which is an extension of pressure correction methods widely used in incompressible flow. In order to validate the new method we compared results from it with the results from the fully explicit code. We observed a good agreement in local instantaneous quantities along with a good agreement in mean quantities for both phases. The relative difference is equal to 1% in the mean gas temperature and 3% in the droplet mean temperature. We also observed a close agreement for such sensitive quantities as droplet size PDF at a single time and the Nusselt number history. This gives an evidence of the overall accuracy of the developed method. A big advantage of the new algorithm, in which the time step is independent of the Mach number, is that it permits to simulate approximately 250 times faster than the old solver for the realistic values of the Mach number $Ma = 0.005$ and for the current flow conditions.

Finally, in Chapter 5 droplet-laden turbulent channel flow with phase transition in the presence of gravity was examined. This additional force leads to the movement of droplets towards the bottom wall where they form a thin film of water. We model the film neglecting its motion and keeping its thickness constant in time. In order to do this we add or drain water near the bottom wall. To have a constant total amount of water on average in the system we also add droplets from the top wall, their diameter is equal to the initial diameter of droplets in the channel. We investigated the mass and heat transfer properties of the two phases such as the mean gas temperature and mean droplet diameter as functions of the wall-normal coordinate in case of an initial number of droplets of 1 million, which are uniformly distributed over the channel. We refer to this case as the reference case. The main findings of the analysis are the development and propagation of a thermal front in the channel and the tendency of the droplets to grow by condensation of vapor on their surface. We analyzed the behavior of droplets and phase transitions by following one droplet, which was inserted at the top wall and considering the evolution of its relevant quantities in time.

Keeping the initial volume fraction constant, we decreased the initial number of droplets to 1/2 million and 1/4 million. We compared the behavior of the droplets in these cases. It was found that in cases of larger initial droplet size droplets tend to fall towards the bottom wall faster and consequently, have smaller residence time in the gas. This results in a smaller growth rate than in the reference case. In addition, we performed a simulation in which we kept the same initial droplet diameter but with initially 2 million droplets. The twice larger initial volume fraction results in a smaller growth rate of droplets because of a lower rate of condensation due to the presence of neighboring droplets. The main conclusion of two performed sets of simulations is that droplets have a large effect on the heat transfer in the channel.

The research presented in this thesis can be continued in three directions. The first direction can be integrated in all four studies presented in Chapters 2, 3, 4 and 5. The second recommendation will help to make the model for the thin film of water at the bottom wall of the channel more complete and going in the third direction will reduce the computational cost in

the simulation of the full model for droplet-laden turbulent channel flow in the presence of gravity.

- In this thesis we considered two-coupling regime of the flow neglecting the droplet-droplet interactions, justifying it by the classification proposed by Elghobashi (1994). Indeed, the initial volume fraction of droplets corresponds to this regime but it is changing with time because of the occurring phase transitions and consequently, four-way coupling may become essential to include. In addition, Vreman et al. (2008) showed that it is necessary to include particle-particle interactions in numerical simulations of turbulent particle-laden channel flow with volume fractions around one percent. Considering droplet-droplet interactions in the system represents physical and numerical challenge. For the modeling we need a criteria which defines whether water droplets bounce or coalesce. From the computation point of view, including four-way coupling can result in expensive simulations at the current volume fractions. The interactions between droplets can be monitored with the procedure proposed by Vreman et al. (2008). For each droplet a list of neighbors is kept which is updated after each collision among the entire droplet swarm. The implementation of this approach or another one needs a special attention caused by the parallel structure of the codes which were used in this thesis.
- The model for the film can be made more complete by introducing several features such as the film movement and the change of the film thickness in time and space. In addition, more sophisticated model can be considered for the film surface since water droplets can be entrapped by the liquid film but they can also be released back because of the turbulent characteristics of the flow in the channel.
- Finally, we would like to perform the simulations described in Chapter 5 more efficiently. This can be achieved through simulations of the full model described in Chapter 5 with the low Mach number code, described in Chapter 4. The wish to use the new solver could lead to the changes in the model for the film since the unknown variables for the carrier phase in the model for the low Mach number solver are not all conservative variables.

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Summary

Multiphase turbulent flows with a large number of dispersed droplets occur frequently in nature and in many industrial applications. Turbulent flow itself presents a complex physical problem and the presence of droplets which can undergo phase transition makes it even more challenging from modeling and numerical points of view. In this thesis we considered the flow of droplets of water in air, in which the presence of water vapor was accounted for. The first question to answer was which formulation to use for the modeling of the carrier phase: compressible or incompressible fluid flow. We performed simulations for the compressible formulation by means of DNS for the carrier phase, using the point-particle approach for the droplets. The numerical model adopts a second-order accurate explicit four-stage low-storage Runge-Kutta time-stepping and a second-order finite volume discretization in space. We confronted the ‘compressible’ results with results of a previous study in which the incompressible formulation was used. The chosen initial conditions are ‘mild’ in the sense of mass transfer: room temperature, atmospheric pressure and 100% initial relative humidity. These initial conditions guarantee a ‘modest’ coupling in mass and energy between the two phases. Moreover, the low Mach number of the test case brings about that the incompressible formulation can be adopted to good approximation for the kinematic and thermal properties of the carrier and dispersed phases. We investigated the sensitivity of the results arising from low-level compressibility effects in this multiphase system. We varied the reference temperature in the channel and the value of the heat flux through the walls. We found that even for the lowest Mach number considered in the compressible formulation the difference in thermal and heat transport properties are significant, e.g., differences in the Nusselt number are on the order 15% when the reference temperature is increased up to 50 degrees C. Despite these differences in heat transport characteristics, the kinematic properties of the flow show good agreement in all cases considered.

The differences in heat transfer properties under mild conditions motivated us to consider more ‘severe’ initial conditions starting from significantly lower values of the initial relative humidity. This has a direct effect during the initial stages when intensive evaporation occurs. We focused on the analysis of the heat transfer properties across the channel walls and found a difference of approximately 25% in the Nusselt number between the compressible and the incompressible formulations in case of an initial relative humidity of 50%. A further analysis showed that this difference is caused by the contribution to the Nusselt number from the droplets.

The explicit time-integration method imposes a severe restriction on the time step arising

from the CFL condition for low values of the Mach number. This motivated us to develop and validate a new time integration method for multiphase flow at low Mach number in which phase transitions play an important role. The general idea is to treat compressible flow with the pressure correction method. As a first step a more suitable system of modeling equations was obtained by means of asymptotic analysis. This system has several advantages: the absence of large eigenvalues which allows to treat most of the terms explicitly and the decomposition of the pressure into two parts: a space-independent thermodynamic part and a hydrodynamic part. The latter feature of the system permits to apply the pressure-correction method to the hydrodynamic part of the pressure. We derived an analytical expression for the divergence of the velocity, which is not equal to zero, taking into account the boundary conditions for channel flow. The main advantage of the new method is the independence of the time step on the Mach number and consequently, a significant gain in calculation time with the new algorithm, which becomes larger at smaller Mach numbers. We estimated that the problem considered can be simulated approximately 250 times faster with the new numerical method than with the fully explicit code for realistic values of the Mach number on the order of 0.005. The results obtained with the two codes show good qualitative and quantitative agreement.

The research presented in the second, third and fourth chapters of this thesis does not take into account gravity. If gravity is in the wall-normal direction of the channel, it would lead to the average movement of droplets towards the bottom wall where a liquid film would form, unless the wall is super-hydrophobic. Hence, as a final step, we included gravity and modeled the film as a thin layer of water of constant height, neglecting its internal motion. Theoretically, the film thickness can change because of evaporation of water from its surface, condensation of water vapor onto it and the direct mass contribution from the droplets falling into the film and merging with it. In order to keep the film thickness constant we drain water from the bottom wall. Simultaneously, we keep the total mass of water in the system constant on average by releasing new water droplets into the channel from the top wall. We describe the film by its energy per unit area and by the film temperature which is approximated using a second order polynomial with coefficients depending on the in-plane coordinates and time. We solve the system of equations for these variables which couples the film, the carrier gas and the droplets. We considered a reference case when initially 1 million droplets were uniformly distributed over the channel. We observed the initial development and propagation of a thermal front in the channel and the tendency of the droplets to grow by condensation of vapor on their surface, while falling down towards the bottom wall.

To understand the effect of droplet size and volume fraction we performed two further sets of simulations. In the first set we kept the initial volume fraction constant and decreased the initial number of droplets to 1/2 million and 1/4 million. Consequently, droplets are initially larger in case of fewer droplets. The droplet behavior was found to be quantitatively different in these two cases compared to the reference case. In cases of larger initial droplet size, the droplets fall towards the bottom wall faster and consequently, have smaller residence time in the gas. This results in a smaller droplet growth. In the second set of simulations the same initial droplet diameter as in the reference case was used, but their initial number was increased to 2 million. The twice larger initial volume fraction results in a somewhat smaller growth of droplets because of a lower rate of condensation due to a 'competition' for vapor arising from the presence of neighboring droplets.

Samenvatting

Turbulente meerfasestromingen waarin een groot aantal deeltjes gedispergeerd zijn komen veelvuldig in de natuur en in industriële toepassingen voor. Turbulente stroming is zonder de aanwezigheid van deeltjes al een complex verschijnsel; de aanwezigheid van deeltjes die faseovergangen kunnen ondergaan maakt het probleem nog uitdagender, zowel voor de fysische als voor de numerieke modellering. In dit proefschrift hebben we de stroming van waterdruppels in lucht met waterdamp bestudeerd. Als eerste hebben we de vraag beantwoord of de gasfase als compressibel gemodelleerd moet worden of dat een incompressibele formulering volstaat. Om die vraag te beantwoorden hebben we simulaties uitgevoerd met een speciaal hiervoor ontwikkelde directe numerieke simulatiemethode voor compressibele stroming van het gas in combinatie met een puntdeeltjesbeschrijving van de waterdruppels. De numerieke methode bestaat uit een tweede-orde nauwkeurige expliciete vierstaps Runge-Kutta methode voor de integratie in de tijd en een tweede-orde eindige volume methode voor de ruimtelijke discretisatie. De resultaten zijn vergeleken met die van een eerder ontwikkelde incompressibele simulatiemethode. In eerste instantie is gekozen voor milde beginvoorwaarden wat de massaoverdracht tussen de twee fasen betreft: kamertemperatuur, atmosferische druk en verzadigde lucht. Hierdoor zijn de koppelingstermen voor energie en massa tussen de twee fasen relatief klein. Het bleek dat zowel voor kinematische als voor thermische eigenschappen van beide fasen de resultaten van beide methodes goed met elkaar overeenkomen. Vervolgens hebben we de gevoeligheid van dit resultaat onderzocht door de simulaties bij hogere temperatuur en bij hogere warmteflux door de wanden uit te voeren. Zelfs bij het laagste Machgetal dat we bekeken hebben zijn de verschillen tussen de resultaten voor thermische en transporteigenschappen van beide formuleringen significant. Zo vonden we bij een begintemperatuur van 50 oC verschillen in het Nusseltgetal in de orde van 15%. De kinematische eigenschappen komen echter nog steeds goed met elkaar overeen in alle bestudeerde testgevallen. De gevonden verschillen bij milde beginvoorwaarden waren de motivatie om deze studie ook uit te voeren bij lagere initiale waterdampconcentratie. Dit leidt in de beginfase tot intensieve verdamping en daardoor tot verschillen in het Nusseltgetal van ongeveer 25% tussen beide formuleringen in het geval dat de initiale relatieve vochtigheid gelijk is aan 50%. Uit analyse van de resultaten bleek dat dit verschil wordt veroorzaakt door de bijdrage van de druppels tot het Nusseltgetal. De gebruikte expliciete tijdtintegratiemethode leidt bij lage Machgetallen tot een sterke restrictie op de tijdstap, die veroorzaakt wordt door de CFL conditie. Daarom hebben we een nieuwe tijdstapmethode ontwikkeld en gevalideerd voor meerfasestroming bij lage Machgetallen waarin faseovergangen een rol spelen. Het basisidee

is om ook voor compressibele stroming een drukcorrectiemethode te gebruiken. Als eerste stap hierin is met behulp van asymptotische analyse voor lage Machgetallen een systeem van vergelijkingen afgeleid dat beter voor deze methode geschikt is. De voordelen van dit systeem zijn het ontbreken van grote eigenwaarden, zodat een expliciete methode gebruikt kan worden voor de meeste termen in de vergelijkingen, en de ontbinding van de druk in een thermodynamisch deel dat onafhankelijk van de plaats is en een hydrodynamisch deel. Door deze ontbinding kan een drukcorrectiemethode toegepast worden voor het hydrodynamische deel van de druk. Hiertoe is met gebruikmaking van de randvoorwaarden een analytische uitdrukking voor de divergentie van de snelheid bepaald, die in dit geval ongelijk is aan nul. Het belangrijkste voordeel van de nieuwe methode is dat voor lage Machgetallen de tijdstap onafhankelijk van het Machgetal gekozen kan worden. Hierdoor ontstaat een grote winst in rekentijd, die toeneemt naarmate het Machgetal kleiner is. Naar schatting is de rekentijd voor ons testgeval bij een realistisch Machgetal van 0.005 een factor 250 kleiner met de nieuwe methode dan met de volledig expliciete methode. De verkregen resultaten van beide methoden komen kwalitatief en kwantitatief goed overeen. Het onderzoek beschreven in hoofdstuk 2-4 van dit proefschrift is uitgevoerd zonder zwaartekracht. Zwaartekracht in de richting loodrecht op de wanden van het kanaal zorgt voor een gemiddelde beweging van druppels naar de onderwand, waar een film zal ontstaan, tenzij deze wand superhydrofoob is. Daarom hebben we als laatste stap in de modelvorming zwaartekracht toegevoegd en een film gemodelleerd als een dunne laag water van constante dikte op de onderwand van het kanaal. De beweging van de film is nog niet verdisconteerd. De filmdikte kan theoretisch veranderen door verdamping van of condensatie op het filmmoppervlak en door druppels die met de film coalesceren. Om toch een constante filmdikte te houden hebben we de juiste hoeveelheid water van de onderwand afgevoerd. Tegelijkertijd is de totale massa water gemiddeld constant gehouden door nieuwe druppels vanaf de bovenwand aan het kanaal toe te voegen. De film is beschreven door zijn energie per eenheid van oppervlakte en door de temperatuur. De temperatuur is benaderd door een tweedegraads polynoom in de loodrechte coördinaat, waarvan de coëfficiënten afhangen van de twee andere coördinaten en van de tijd. Vervolgens wordt het systeem van vergelijkingen voor deze variabelen, dat film, gas en druppels aan elkaar koppelt, opgelost. Als referentiegeval hebben we een probleem met initieel een miljoen druppels die uniform over het kanaal verdeeld zijn gekozen. Voor dit geval hebben we de initiele ontwikkeling en beweging van een thermisch front in het kanaal gezien, alsmede de tendens dat druppels groeien door condensatie van waterdamp op hun oppervlak, terwijl ze naar de onderwand toe bewegen. Om het effect van de druppelgrootte en volumefractie te begrijpen hebben we twee andere reeksen van simulaties gedaan. In de eerste reeks hebben we bij constante volumefractie het initiele aantal druppels verlaagd tot een half miljoen en een kwart miljoen. Een kleiner aantal druppels betekent dat hun beginafmeting groter is. Vergeleken met het referentiegeval is een kwalitatief ander gedrag van de druppels waargenomen. Een grotere druppel leidt namelijk tot een grotere valsnelheid en daardoor een kleinere verblijftijd in het kanaal. Daardoor groeien de druppels minder snel. In de tweede reeks van simulaties werd de druppelgrootte hetzelfde genomen als in het referentiegeval, maar is het initiele aantal verhoogd tot twee miljoen. Dit resulteert in een enigszins kleinere druppelgroei, omdat de condensatiesnelheid lager is vanwege het feit dat meer druppels met elkaar in competitie zijn voor dezelfde hoeveelheid waterdamp.

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About the author

Anastasia Bukhvostova was born on the 25th of April 1989 in Moscow, Russia. She graduated with honors from the Lyceum 1580 of Moscow with specialization in mathematics and physics in 2006. She continued her education entering the Mechanics and Mathematics Department of Lomonosov Moscow State University. In September 2008 she chose to specialize in the dynamics of gas and waves and she graduated with honors in June 2011 with her Master thesis 'Oscillator with non-potential repulsion' written under the supervision of associate professor B.V. Kuksenko. After obtaining her Master degree she was accepted as a PhD candidate in the FOM project 'Droplets in Turbulence'. She worked under the supervision of professors Bernard Geurts and Hans Kuerten. The results of her work are presented in this thesis. During the four years of this project she participated in several conferences which helped her to broaden her scientific network and obtain experience in presenting results. The results were also reported in several published papers. She assisted in a numerical course on numerical mathematics for bachelor students.

List of publications

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