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

A. Bukhvostova a,* , E. Russo b , J.G.M. Kuerten a,b , B.J. Geurts a,c

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.

© 2014 Elsevier Inc. All rights reserved.

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 Mashayek (1997) 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 Masi et al. (2010) investigated the interaction of a non-isothermal droplet-laden turbulent planar 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., 2014). 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. (2014) 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., 2014). 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 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. The differences in the behavior of the system under different initial conditions are discussed in Section 4. A comparison of the results from the two formulations is presented in Section 5. Finally, concluding remarks are collected in Section 6.

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 for these cases.

The organization of this paper is as follows. In Section 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. The differences in the behavior of the system under different initial conditions are discussed in Section 4. A comparison of the results from the two formulations is presented in Section 5. Finally, concluding remarks are collected in Section 6.

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 Fig. 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):

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

$$\partial_t (\rho u_j) + \partial_j (\rho u_j u_i) = -\partial_j \tau_{ij} + F_i + Q_{mom,i} \quad (2)$$

$$\partial_t e_i + \partial_j (\rho u_j e_i) = -\partial_j q_j - \partial_j (u_i \tau_{ij}) + Q_e \quad (3)$$

$$\partial_t (\rho Y_v) + \partial_j (\rho u_j Y_v) = -\partial_j j_v + Q_m \quad (4)$$

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, $(\rho, u_i, e, Y_v)$ are the carrier phase mass density, components of the velocity, total energy density and vapor mass fraction, respectively. Moreover, $\tau_{ij}$ 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 $\mu$. In fact, we adopt the Sutherland law for the dynamic viscosity $\mu$ (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 3 K. It was found in Bukhvostova et al. (2014) 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 differences between the walls of up to 40 K, as studied, e.g., by Zonta and Soldati (2014), inclusion of the temperature dependency of $K, D$ and $\mu$ 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 Eqs. (1)–(4) is made non-dimensional using a set of reference scales of the system as will be further specified in Section 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.

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 \((\rho, \mathbf{u}, T, \rho Y_v)\):

\[
\nabla \cdot \mathbf{u} = 0
\]

\[
\rho \left( \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla P + \rho \mathbf{F} + \mathbf{L}_u
\]

\[
\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\mathbf{u} \rho \mathbf{u}) = \frac{\partial P}{\partial t} + \nabla \cdot (P\mathbf{F}) + \mathbf{L}_u
\]

\[
\begin{align*}
\hat{c}_p &= \rho (1 - Y_v) c_{p,g} + \rho Y_v c_{p,v} \\
\end{align*}
\]

where \(c_{p,g}\) and \(c_{p,v}\) are the specific heats of air and water vapor, respectively.

The term \(\mathbf{F}\) expresses the momentum exchange between the two phases. Moreover, \(\mathbf{L}_u\) stands for the heat capacity at constant volume of the air–water vapor mixture.

\[
\begin{align*}
\hat{c}_v &= \rho \left( 1 - Y_v \right) c_{v,g} + \rho Y_v c_{v,v} \\
\end{align*}
\]

The equation for the vapor mass density is the same as in the compressible formulation. In (6) \(\omega\) stands for the vector of vorticity \(\omega = \nabla \times \mathbf{u}\), \(P = p_g + \frac{1}{2} \rho \mathbf{u}^2\), \(\mu\) is the dynamic viscosity of the gas, \(p_g\) 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 \(\mathbf{L}_u\) 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:

\[
\begin{align*}
\hat{c}_v &= \rho (1 - Y_v) c_{v,g} + \rho Y_v c_{v,v} \\
\end{align*}
\]

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:

\[
\begin{align*}
d\mathbf{x}_i(t) = \mathbf{v}_i \\
\end{align*}
\]

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):

\[
\begin{align*}
\frac{d\mathbf{v}_i}{dt} = \frac{\mathbf{u}(\mathbf{x}_i, t) - \mathbf{v}_i}{\tau_{di}} - \left( 1 + 0.15 \text{Re}_{di}^{0.87} \right) \frac{\mathbf{v}_i}{\tau_{di}} \\
\end{align*}
\]

where \(\mathbf{u}(\mathbf{x}_i, t)\) is the velocity of the carrier gas at the droplet position. Moreover, \(\tau_{di} = \rho_i d_i^2/(18\mu)\) defines the droplet relaxation time where \(\rho_i\) and \(d_i\) stand for liquid water mass density and droplet diameter of droplet \(i\), respectively. In addition, \(\text{Re}_{di}\) 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:

\[
\text{Re}_{di} = \frac{d_i \rho_i |\mathbf{u}(\mathbf{x}_i, t) - \mathbf{v}_i|}{\mu}
\]

Next to the change of droplet velocity and position we also take into account how its energy, given by \(E_i = c_m T_i\), changes in time. Here, \(c_i\) 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:

\[
\begin{align*}
\frac{d}{dt} E_i = h_{dl}(\mathbf{x}(\mathbf{x}_i, t) - T_i) \\
\end{align*}
\]

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

\[
\begin{align*}
h_{dl} d_i^2 &= 2 + 0.60 \text{Re}_{di}^{1/2} \text{Pr}^{1/3} \\
\end{align*}
\]

Finally, \(A_i\) denotes the surface area of droplet \(i\) and \(T(\mathbf{x}, t)\) 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, p. 711):

\[
\begin{align*}
\frac{dm_i}{dt} = - \frac{m_i \text{Sh}_{di}}{3 \tau_{si} \text{Sc}} \ln \left( \frac{1 - \text{Y}_{i,pl}}{1 - \text{Y}_{i,s}} \right) \\
\end{align*}
\]

where \(Y_{i,pl}\) and \(Y_{i,s}\) are the vapor mass fractions at a distance \(\delta\) 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 \(\delta\). For the Sherwood number of a droplet we use the correlation for a sphere (Bird et al., 1960):

\[
\text{Sh}_{di} = 2 + 0.60 \text{Re}_{di}^{1/2} \text{Sc}^{1/3}
\]

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

\[
\begin{align*}
p_{v,sat} &= 10^A \exp \left( \frac{B - C \text{K}}{T + T_i} \right) \\
\end{align*}
\]

where \(A = 11.6834, B = 4089.59\) K and \(C = 500.02\) K and \(T_i\) is taken in Kelvin, in combination with the ideal gas law for water vapor while \(Y_{i,pl}\) 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 (Bukhvostova et al., 2014). For example, the two-way coupling term in continuity Eq. (1) and in total energy density Eq. (3) are given by expression:

\[
\begin{align*}
Q_m = - \sum_i \frac{dm_i}{dt} \delta(\mathbf{x} - \mathbf{x}_i) \\
Q_e = - \sum_i \frac{d}{dt} \left( c_m T_i \delta(\mathbf{x} - \mathbf{x}_i) \right)
\end{align*}
\]

<table>
<thead>
<tr>
<th>Case</th>
<th>RH100</th>
<th>RH75</th>
<th>RH50</th>
</tr>
</thead>
<tbody>
<tr>
<td>(T_{sat}) (K)</td>
<td>293.15</td>
<td>293.15</td>
<td>293.15</td>
</tr>
<tr>
<td>(\rho_{v,sat}(T_{sat})) (kg/m(^3))</td>
<td>0.0169</td>
<td>0.0127</td>
<td>0.0085</td>
</tr>
<tr>
<td>(\rho_{v}(kg/m^3))</td>
<td>1.194</td>
<td>1.8998</td>
<td>1.1855</td>
</tr>
<tr>
<td>(u_b(m/s))</td>
<td>1.8246</td>
<td>1.8311</td>
<td>1.8377</td>
</tr>
<tr>
<td>(Re_{di})</td>
<td>2333</td>
<td>2333</td>
<td>2333</td>
</tr>
<tr>
<td>(Ma)</td>
<td>0.05</td>
<td>0.05</td>
<td>0.05</td>
</tr>
<tr>
<td>(Pr)</td>
<td>0.7425</td>
<td>0.7395</td>
<td>0.7365</td>
</tr>
<tr>
<td>(Sc)</td>
<td>0.62883</td>
<td>0.63055</td>
<td>0.6328</td>
</tr>
</tbody>
</table>

Table 1: Parameters of the test cases.
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.

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 Eqs. (1)–(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. 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 (1)–(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 \( u_{\text{ref}} \) which is taken as the initial bulk velocity of the carrier gas:

\[
 u_{b} = \frac{Re_b \mu(T_{\text{ref}})}{L \rho_{\text{ref}}} \tag{19}
\]

where the reference temperature \( T_{\text{ref}} \) is chosen to be equal to 293.15 K and the dynamic viscosity at the reference temperature \( \mu(T_{\text{ref}}) \) 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 \( H = 2 \text{ cm} \). The reference mass density \( \rho_{\text{ref}} \) 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 \( \phi \) 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 \( p_{v,sat}(T_{\text{ref}}) \) using Antoine’s relation (16). Consequently, we know the partial pressure of water vapor which is equal to \( \phi p_{v,sat}(T_{\text{ref}}) \). From the equation of state for water vapor we may find the initial vapor mass density \( \rho_v(T_{\text{ref}}) \) in the channel corresponding to the chosen relative humidity:

\[
 \rho_v(T_{\text{ref}}) = \rho_Y(T_{\text{ref}}) = \frac{\phi p_{v,sat}(T_{\text{ref}})}{R_{\text{water}} T_{\text{ref}}} \tag{20}
\]

where \( R_{\text{water}} \) denotes the specific gas constant of water. We vary the initial \( \phi \) in this study, choosing values of 100%, 75% and 50%. These cases will be called RH100, RH75 and RH50, respectively. In Table 1 the initial vapor mass density \( \rho_v(T_{\text{ref}}) \) at the reference temperature is shown.

In (19) the reference density \( \rho_{\text{ref}} \) 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:

\[
 p = R_{\text{air}} \rho_{\text{air}} T_{\text{ref}} + R_{\text{water}} \rho_v(T_{\text{ref}}) T_{\text{ref}} \tag{21}
\]

where \( R_{\text{air}} \) stands for the specific gas constant of dry air. In addition, \( \rho_{\text{air}} \) and \( \rho_v \) define the mass density of dry air and water vapor, respectively. We express the mass density of pure air from (21):

\[
 \rho_{\text{air}} = \frac{p - R_{\text{water}} \rho_v(T_{\text{ref}}) T_{\text{ref}}}{R_{\text{air}} T_{\text{ref}}} \tag{22}
\]

Knowing \( \rho_v(T_{\text{ref}}) \) from (20), we can find the initial mass density of dry air and, consequently, the initial mass density of the mixture:

\[
 \rho = \rho_{\text{air}} + \rho_v(T_{\text{ref}}) \tag{23}
\]

Table 1 shows the reference mass density. Because of the different initial amount of water vapor in the mixture, \( \rho_v(T_{\text{ref}}) \), the reference mass density is different in each case. Consequently, it leads to different initial bulk velocities as it is seen from (19).

The Mach number depends on the Reynolds number and it is calculated according to:
Ma \ = \ \frac{u_{ref}}{c(T_{ref})} = \frac{R_{air} \mu(T_{ref})}{T_{ref} \rho_{air} c(T_{ref})} \tag{24}

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

\[
c(T_{ref}) = \sqrt{\gamma_{air} R_{air} T_{ref} / M_{air}} \tag{25}
\]

where \( \gamma_{air} \) 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 (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 \( Ma = 0.05 \). In (Bukhvostova et al., 2014) it was shown that at this Mach number all gas and droplets characteristics that would arise at \( Ma = 0.005 \) are accurately approximated.

The other non-dimensional parameters of the simulations are shown in Table 1. The Prandtl number is defined in the following way:

\[
Pr = \frac{c_{pa} \mu(T_{ref})}{K(T_{ref})} \tag{26}
\]

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, p. 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:

\[
Sc = \frac{\mu(T_{ref})}{\rho_{ref} D(T_{ref})} \tag{27}
\]

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 \( \rho_{ref} \) in (27) leads to different values of the Schmidt number in the three cases considered.

We randomly distribute \( N_{drop} = 2,000,000 \) 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 \( 1.9 \times 10^{-4} \) 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.

### 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, Fig. 2. The figure confirms what is predicted by (14). The driving force in (14) is the difference \( Y_{\beta,\beta} - Y_{\beta,s} \). For an unsaturated initial condition \( Y_{\beta,\beta} \) is smaller than \( Y_{\beta,s} \) and this leads to negative values of \( \frac{d_{\beta,s}}{d_{\beta,\beta}} \). The smaller initial relative humidity leads to a smaller value of \( Y_{\beta,s} \) and, consequently, to a more negative \( \frac{d_{\beta,s}}{d_{\beta,\beta}} \). 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.
The behavior of the relative humidity as a function of time is connected to the behavior of the droplets, Fig. 3. The behavior of the relative humidity can also be predicted analytically to a good approximation. For that we may reason as follows. Combining Eqs. (1) and (4), we obtain the equation for the vapor mass fraction change:

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

(28)

The convective and diffusive terms in (28) can be neglected since the initial conditions lead to a small gradient of the vapor mass fraction so that the source term in (28) is dominant. The typical values of $Y_v$ are small compared to 1, Table 1. Consequently, the behavior of $Y_v$ is well approximated by:

$$\frac{dY_v}{dt} = \frac{Q_m}{\rho}$$

(29)

Substituting two-way coupling term (17) and using a Taylor expansion for $\ln \left(\frac{1 - Y_{v,s}}{1 - Y_v}\right)$ in Eq. (14) we obtain:

$$\frac{dY_v}{dt} = Y_{v,s} - Y_{v,s}$$

(30)

where $\tau$ stands for the evaporation relaxation time which is equal to:

$$\tau = \frac{3\tau_{sd} \rho Sc V}{m_{sd} N_{drop}}$$

(31)

We divide Eq. (30) by the saturation vapor mass fraction $Y_{v,s}$ and obtain an equation for the change of the relative humidity:

$$\frac{d\phi}{dt} = \frac{1 - \phi}{\tau}$$

(32)

For our initial conditions we obtain $\tau = 0.0658$ s. The insert in Fig. 3a shows the analytical solution of (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.

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.

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 Fig. 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, Fig. 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 Fig. 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 Eq. (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 Eq. (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,Fig. 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, Fig. 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 $Q_{\text{m}}$ in Eq. (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.

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, Fig. 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, Fig. 7c. The equation for the carrier gas temperature change is Eq. (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 $h_m A_i (T(x, t) - T_i)$. We verified with the compressible solver in case RH100 that this term has on average a twice larger absolute value than the term $h_v \frac{\partial T}{\partial y}$ in Eq. (14). The exchanged energy between the two phases $h_m A_i (T(x, t) - T_i)$ causes a change in energy of the carrier gas quantified by $c_p V \rho \frac{\partial T}{\partial y}$, where $c_p$ 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, Fig. 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:

$$\text{Nu} = \frac{\left(\frac{d(T)}{dy}_{\text{wall}}\right)_w}{\Delta(T) / 2H}$$

where $\Delta(T)$ 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. Fig. 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 $[2 \text{ s}; 5 \text{ s}]$ is 1.5 times larger in RH50 than in RH100, Table 2.

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

$$\text{Nu} = \text{Nu}_{\text{lam}} + \text{Nu}_{\text{turb}} + \text{Nu}_{\text{part}},$$

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

<table>
<thead>
<tr>
<th></th>
<th>RH50</th>
<th>RH100</th>
</tr>
</thead>
<tbody>
<tr>
<td>Compr</td>
<td>13.91</td>
<td>15.53</td>
</tr>
<tr>
<td>Incompr</td>
<td>13.04</td>
<td>14.83</td>
</tr>
</tbody>
</table>
are negligible (Russo et al., 2014). We calculated all three contributions in (34) in cases RH100, RH75 and RH50 in the incompressible formulation, Table 3, averaging over time interval [2 s; 5 s]. The difference in the resulting Nusselt number between cases RH100 and RH50 is caused by a relative difference on the order of 10% in $\text{Nu}_{\text{part}}$ while the other contributions are virtually unchanged. In Kuerten et al. (2011) a simplified expression for $\text{Nu}_{\text{part}}$ is given:

$$
\text{Nu}_{\text{part}} = - \int_{-H}^{H} \int_{-H}^{H} \frac{2\pi n(s) \langle \Delta T \rangle}{\langle \Delta T \rangle_{t}} dy ds,
$$

(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 (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 $\frac{T(x_i, t) - T_{\text{wall}}}{T_{\text{wall}}}$, 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, Fig. 9a and b, the normalized

<table>
<thead>
<tr>
<th>Case</th>
<th>$\text{Nu}$</th>
<th>$\text{Nu}_{\text{lam}}$</th>
<th>$\text{Nu}_{\text{turb}}$</th>
<th>$\text{Nu}_{\text{part}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>RH100</td>
<td>14.5</td>
<td>1.0</td>
<td>2.5</td>
<td>11.0</td>
</tr>
<tr>
<td>RH75</td>
<td>14.2</td>
<td>1.0</td>
<td>2.6</td>
<td>10.6</td>
</tr>
<tr>
<td>RH50</td>
<td>13.4</td>
<td>1.0</td>
<td>2.6</td>
<td>9.8</td>
</tr>
</tbody>
</table>

Table 3
Contributions in the Nusselt number for cases RH100, RH75 and RH50. Time averaging is performed for the time interval [2 s; 5 s].
relative temperature is quite different, especially in the regions near the walls, Fig. 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 5 K. 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, Fig. 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. Fig. 10 illustrates in a more detailed way Fig. 2. Droplets evaporate more in RH50 than in RH100 at 0.1 s as Fig. 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.

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. Figs. 2, 4b and 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.

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 number 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.

References