Weierstraß-Institut
für Angewandte Analysis und Stochastik
Leibniz-Institut im Forschungsverbund Berlin e. V.

Preprint ISSN 0946 – 8633

On balance laws for mixture theories of disperse vapor bubbles in liquid with phase change

Wolfgang Dreyer[1], Maren Hantke[2], Gerald Warnecke[2]

submitted: 5th November 2012

[1] Weierstrass Institute
Mohrenstr. 39
10117 Berlin
Germany
E-Mail: wolfgang.dreyer@wias-berlin.de

[2] Institute for Analysis and Numerics
Otto-von-Guericke-University Magdeburg
PSF 4120
39016 Magdeburg
Germany
E-Mail: maren.hantke@ovgu.de
gerald.warnecke@ovgu.de

No. 1741
Berlin 2012

2010 *Mathematics Subject Classification.* 35Q53, 35G25, 76E15.

Key words and phrases. Averaging methods, conservation laws, phase change, bubbles, phase mixtures.

We gratefully acknowledge that the work of the authors was partially supported by the Deutsche Forschungsgemeinschaft (DFG) grant Wa 633/17-2 in the DFG-CNRS French-German research group FOR 563 *Micro-macro Modeling and Simulation of Liquid-Vapor Flows.* Wolfgang Dreyer would like to thank the German Research Foundation (DFG) for financial support of the project *Modeling and sharp interface limits of local and non-local generalized Navier- Stokes-Korteweg Systems.*

Edited by
Weierstraß-Institut für Angewandte Analysis und Stochastik (WIAS)
Leibniz-Institut im Forschungsverbund Berlin e. V.
Mohrenstraße 39
10117 Berlin
Germany

Fax: +49 30 2044975
E-Mail: preprint@wias-berlin.de
World Wide Web: http://www.wias-berlin.de/

Abstract

We study averaging methods for the derivation of mixture equations for disperse vapor bubbles in liquids. The carrier liquid is modeled as a continuum, whereas simplified assumptions are made for the disperse bubble phase. An approach due to Petrov and Voinov is extended to derive mixture equations for the case that there is a phase transition between the carrier liquid and the vapor bubbles in water. We end up with a system of balance laws for a multi-phase mixture, which is completely in divergence form. Additional non-differential source terms describe the exchange of mass, momentum and energy between the phases. The sources depend explicitly on evolution laws for the total mass, the radius and the temperature of single bubbles. These evolution laws are derived in a prior article [4] and are used to close the system. Finally numerical examples are presented.

1 Introduction

The aim of the paper is to derive mixture balance laws for fluid flows with phase transition. We derive balance laws for mass and momentum as a first step. Analogously, we derive balances for the energy of the phases.

We are considering a mixture of a disperse phase of small ball shaped bubbles of water vapor, immersed in a carrier fluid of the corresponding other liquid phase. The advantage of considering a dispersed phase is that one may use a simpler specific averaging technique to describe it. In a more general approach for two phase mixtures one would use for both phases the averaging that we use only for the carrier fluid.

There are many techniques available to go from some microscopic modeling to macroscopic models. All of them involve a form of averaging in some sense. There is the theory of homogenization which mostly considers periodic structures, see Bensoussan et al. [3], and does the averaging by considering weak limits of periodically fluctuating physical states. There are the methods of moments, which may be seen as weighted global averages, such as those described in Müller and Ruggieri [14] or local averaging techniques such as those we want to consider. There are a number of such local averaging techniques, namely ensemble averaging, time averaging and spatial averaging, see Drew and Passman [5]. Also we want to mention Ishii [10], Stewart and Wendroff [19], Nigmatulin [16] among many other publications. All forms of averaging lead to the same type of macroscopic equations. We pursue spatial averaging.

It is not too difficult to arrive at averaged equations, but most approaches lead to additional variables which need closure relations in the form of state equations. This is not so surprising, since most theories at the level of continuum mechanics need such closure relations to completely determine the mathematical model equations. In the case we consider here, already the microscopic equations for the continuous phase used for the averaging come with equations of state.

There are also some numerical techniques along this line, see for instance Engquist and Hou [6].

Our approach is based on volume averaging techniques due to Voinov and Petrov [23] for the same problems which were studied in detail in a diploma thesis of Rydzewski [17]. In our approach we aim at taking the compressible Euler equations to describe the microscopic flow in the carrier phase whereas Voinov and Petrov [23, 24, 22] assumed a potential flow field and made explicit use of the known solution of potential flow around a sphere. Our results are therefore more general than those. But we do take up the idea to use a potential flow in order to determine the interfacial terms on the spherical surfaces between the phases. The remarkable difference to other two phase models is, that our model is completely in divergence form.

We average by using a type of sliding average over a ball of radius $a > 0$ in space. The diameter of the ball $d = 2a$ is the scale at which we want to derive macroscopic equations for the mixture of a liquid phase L occupying most of the space and a dispersed phase consisting of bubbles B consisting of small balls with radii considerably smaller than a.

This averaging is a specific case of volume averaging as described in Drew and Passman [5], though our notation is different and taken from Voinov and Petrov [23]. Drew and Passman argue at the end of Chapter 10 that ensemble averaging, i.e. an approach of statistical physics, is the preferred form of averaging to be used for multi-component fluids. We believe that we are considering a mere change of scale and therefore a fixed scale d introduced by the size of the balls is more adequate to describe the micro-macro transition in modeling. We are assuming that we have a deterministic microscopic model with a given unique dynamics, though existence and uniqueness currently cannot be proven mathematically rigorously for the model equations we are using.

For the microscopic phases we assume that they are not in equilibrium with each other and we want to focus on modeling their interacting dynamics including phase changes between them.

The paper is organized as follows. In Section 2 we introduce the averaging procedures and obtain meaningful averaged quantities. We prove a bubble and a general transport theorem. In the next section we derive balance laws for the carrier and the dispersed phase. In Section 4 we obtain closure relations for the sources to describe the exchange of mass, momentum and energy between the phases. In Section 5 we give some mathematical properties of a radial symmetric submodel. We recall the evolution laws obtained in [4] in Section 6 and give some numerical examples in Section 7. Finally, some detailed calculations for the proofs can be found in the appendix.

2 Local spatial averaging techniques

We assume that the space $\mathbb{R}^3$ contains a mixture of two separated fluids. In this study we consider an ensemble of $\mathscr{N}$ bubbles immersed in a liquid, thus forming the dispersed phase resp. the carrier phase. Further we require that the number of bubbles is constant. In order to take care of nucleation and dissolution of bubbles, we allow for bubbles with zero radius. The merging or breakage of bubbles are excluded in our approach since this would require an additional evolution law for the number of bubbles. The number $\mathcal{N}$ thus gives the maximal number of real bubbles in the system.

Both phases are represented here by different types of averaging operators. Mean values of properties of the dispersed phase consisting of bubbles, indicated by B, are given by sums over the bubbles, whereas in the liquid, indicated by L, we will have integrals over the liquid domain.

For the averaging we take a ball $B_a(0)$ of radius $a > 0$ at the origin, i.e. for a general ball we set $B_a(\mathbf{x}) = \{\mathbf{x}' \in \mathbb{R}^3 \mid |\mathbf{x}' - \mathbf{x}| < a\}$, and denote its volume by $V_a = \frac{4\pi}{3}a^3$. Thereby we define the volume averaging characteristic function or *window function*

$$\chi_a(\mathbf{x}) = \begin{cases} \frac{1}{V_a} & \mathbf{x} \in B_a(0) \\ 0 & \text{otherwise.} \end{cases}$$

Note that by standard smoothing techniques with Friedrichs mollifiers one could also take a smoothed approximation of the characteristic function over $B_a(0)$. If we consider derivatives of non-smooth functions to be taken in the sense of distributions we may avoid this. Either way, it should be noted that there is a mathematical theory making all the arguments below completely rigorous, but care has to be taken in each step. Since we want to concentrate on basic properties of the resulting system of differential equations, we leave out these technical details. They would only obscure the theory without giving additional insight.

Further, we assume that any bounded subset of $\mathbb{R}^3$ contains at most finitely many balls $B_\alpha(t)$ of radius $R_\alpha(t) > 0$ with $R_\alpha(t) \ll a$, with midpoints at $\mathbf{q}_\alpha(t) \in \mathbb{R}^3$, and volume $V_\alpha(t)$, i.e. $B_\alpha(t) = \{\mathbf{x} \in \mathbb{R}^3 \mid |\mathbf{x} - \mathbf{q}_\alpha(t)| < R_\alpha(t)\}$ and $V_\alpha(t) = \frac{4\pi}{3}R_\alpha(t)^3$. Let $\boldsymbol{\eta}_\alpha$ be the vector field of outer unit normals to the surface of $B_\alpha(t)$. To describe the surface points of the balls, we introduce the radial vectors $\mathbf{R}_\alpha(t,\boldsymbol{\eta}_\alpha) = R_\alpha(t)\boldsymbol{\eta}_\alpha$ such that the points $\mathbf{q}_\alpha(t) + \mathbf{R}_\alpha(t,\boldsymbol{\eta}_\alpha)$ lie on the surface of the respective ball. For the surface area we set $O_\alpha(t) = 4\pi R_\alpha(t)^2$. We denote by $m_\alpha(t)$ the mass of the ball $B_\alpha(t)$, by $\mathbf{v}_\alpha(t) = \dot{\mathbf{q}}_\alpha(t)$ the velocity of its midpoint, by $\mathbf{w}_\alpha(t,\boldsymbol{\eta}_\alpha) = \dot{\mathbf{q}}_\alpha(t) + \dot{\mathbf{R}}_\alpha(t,\boldsymbol{\eta}_\alpha)$ the velocity of its boundary, and by $\rho_\alpha(t) = m_\alpha(t)/V_\alpha(t)$ its mass density. For notational convenience we will not always explicitly write out the dependence of the radial vectors and velocities on the unit normals.

The balls just described contain solely the dispersed bubbles B whereas their complement $\Omega_L(t)$

$$\Omega_L(t) = \mathbb{R}^3 \setminus \bigcup_\alpha B_\alpha(t)$$

is filled completely with only the carrier fluid L. Then we define the *volume fraction* of the disperse phase as

$$c(t,\mathbf{x}) = \sum_\alpha \chi_a(\mathbf{x} - \mathbf{q}_\alpha(t))V_\alpha(t). \tag{1}$$

The sum is finite for each $\mathbf{x} \in \mathbb{R}^3$ and is taken over all small balls containing the dispersed phase that have their midpoint within a distance a of $\mathbf{x}$. The volume fraction of the carrier fluid is then set to be $1 - c(t,\mathbf{x})$ in order to preserve volume. These volume fractions are step functions, i.e. not smooth.

Note that we are purposely making a small error by taking the full volume of any ball with its center in $B_a(\mathbf{x})$, even if it is not contained completely in $B_a(\mathbf{x})$. At the same time we neglect the volume of some balls that have their center outside and cut it. Otherwise we could have replaced in (1) $V_\alpha(t)$ by the volume measure $|B_\alpha(t) \cap B_a(\mathbf{x})|$. This would add a notational complication to the averaging formula of the dispersed phase without leading to any substantial changes in the outcome of the averaging. Note that our definition implies that the function c is not continuous where the midpoint of a dispersed phase ball $B_\alpha(t)$ leaves or enters the averaging ball $B_a(\mathbf{x})$.

The dispersed phase is assumed to consist of well separated very small balls. We are aware that in reality a dynamic dispersed phase will not come in spherical shapes, but do not wish to complicate the averaging procedure unnecessarily at this point. So we further assume for simplicity that certain physical properties Ψ, namely density, pressure and temperature are spatially constant and only time dependent within each ball, but may be different in neighboring balls. Note that the velocity must then be radially dependent in order to guarantee local mass conservation. We generically denote these quantities by $\Psi_\alpha(t)$. In the carrier fluid any field quantity Ψ depends on t and the spatial point $\mathbf{x}' \in \Omega_L(t)$.

Next we define the spatial *liquid average* for extensive physical variables by

$$(1-c)\overline{\Psi}(t,\mathbf{x}) = \int_{\Omega_{L(t)}} \Psi(t,\mathbf{x}')\, \chi_a(\mathbf{x}-\mathbf{x}')\, d\mathbf{x}'. \tag{2}$$

Extensive variables describe those quantities that double in case the system size is doubled. In case that no bubble is cut by the averaging ball B_a, this is equivalent to the definition

$$\overline{\Psi}(t,\mathbf{x}) = \frac{\int_{\Omega_{L(t)}} \Psi(t,\mathbf{x}')\, \chi_a(\mathbf{x}-\mathbf{x}')\, d\mathbf{x}'}{\int_{\Omega_{L(t)}} \chi_a(\mathbf{x}-\mathbf{x}')\, d\mathbf{x}'} \tag{3}$$

In this study we need both averages, where (2) is used for establishing the evolution equation, while (3) is more convenient for numerical calculations.

Correspondingly we define the spatial *average of the dispersed phase* for extensive physical variables as

$$c\,\overline{\Psi_\alpha}(t,\mathbf{x}) = \sum_\alpha \Psi_\alpha(t)\, \chi_a(\mathbf{x}-\mathbf{q}_\alpha(t))V_\alpha(t). \tag{4}$$

Note that the form of spatial averaging in (4) is somewhat different from taking (2) and assuming that Ψ has piecewise constant values Ψ_α on subsets of volume V_α containing representative points $\mathbf{x}' = \mathbf{q}_\alpha$. The spatial average (4) leads to step functions whereas the integration in (3) leads to continuous functions in this case. Also there is a slight deviation due to the fact that (4) is taken only over the balls with at least their center point in $B_a(\mathbf{x})$ and we take their full volume, not just their intersection with $B_a(\mathbf{x})$ as a precise application of (2) would require. On the other hand balls with an intersection having their center outside the averaging domain are completely neglected. This small error is carried through all the arguments. It does not have any influence on the form of the averaged equations to be derived. There is only an imprecision for quantitative predictions. Also note, that our averaging procedure is similar to, but slightly different from the procedure in the book of Nigmatulin [16, p. 28], who also uses spatial averaging techniques.

Further, we point out that in the spatial averaging (2) we do not have the property $\overline{\overline{\Psi}} = \overline{\Psi}$. The double average involves integration over a ball or radius $2a$. Such a property is only true for ensemble averages or periodic functions averaged over their periods. For our discrete average (4) a double average is not meaningful because it gives a density that is independent of α. We only use the notation $\overline{\Psi_\alpha}$ to point out that the averaged variable is related to the dispersed balls. Microscopic quantities for the carrier fluid have no index.

Quantities related to the interfaces

$$I_\alpha(t) = \partial B_\alpha(t) = \{\mathbf{x} \in \mathbb{R}^3 \mid \ |\mathbf{x} - q_\alpha(t)| = R_\alpha(t)\}$$

will have an index I_α.

Next we consider special choices for the properties Ψ_α resp. Ψ for the bubbles and the liquid. The only meaningful choices are densities of additive quantities. See Section 4 for more details. Note that Nigmatulin [16] did not discuss this point

The simplest choice is $\Psi_\alpha \equiv 1$. This results in representation (1) of the concentration of the bubbles which is the local mean value of their volumes. The mean values of m_α/V_α, $1/V_\alpha$, $m_\alpha \dot{q}_\alpha/V_\alpha$ and $m_\alpha e_\alpha/V_\alpha$ give the mass density ρ_B, the number density n, the momentum density $\rho_B v_B$ and the total energy density $\rho_B e_B$ of the bubbles. The latter is assumed to be the sum of the internal and the kinetic energy

$$\begin{aligned}
c\rho_B(t,\mathbf{x}) &= \sum_\alpha m_\alpha(t)\, \chi_a(\mathbf{x} - \mathbf{q}_\alpha(t)), & (5)\\
cn(t,\mathbf{x}) &= \sum_\alpha \chi_a(\mathbf{x} - \mathbf{q}_\alpha(t)), & (6)\\
c\rho_B \mathbf{v}_B(t,\mathbf{x}) &= \sum_\alpha m_\alpha(t)\dot{\mathbf{q}}_\alpha(t)\, \chi_a(\mathbf{x} - \mathbf{q}_\alpha(t)), & (7)\\
c\rho_B e_B(t,\mathbf{x}) &= \sum_\alpha m_\alpha(t) e_\alpha(t)\, \chi_a(\mathbf{x} - \mathbf{q}_\alpha(t))\,. & (8)
\end{aligned}$$

In the liquid we only have to define the mass density, the momentum density and the total energy density by the corresponding formulas

$$\begin{aligned}
(1-c)\rho_L(t,\mathbf{x}) &= \textstyle\int_{\Omega_{L(t)}} \rho(t,\mathbf{x}')\, \chi_a(\mathbf{x} - \mathbf{x}')\, d\mathbf{x}', & (9)\\
(1-c)\rho_L \mathbf{v}_L(t,\mathbf{x}) &= \textstyle\int_{\Omega_{L(t)}} \rho(t,\mathbf{x}')\mathbf{v}(t,\mathbf{x}')\, \chi_a(\mathbf{x} - \mathbf{x}')\, d\mathbf{x}'\,, & (10)\\
(1-c)\rho_L e_L(t,\mathbf{x}) &= \textstyle\int_{\Omega_{L(t)}} \rho(t,\mathbf{x}') e(t,\mathbf{x}')\, \chi_a(\mathbf{x} - \mathbf{x}')\, d\mathbf{x}'\,. & (11)
\end{aligned}$$

Note that now we have at each point in space a partial density $c\rho_B$ of the bubbles and a partial density $(1-c)\rho_L$ of the liquid. The same is true for the momentum and the energy. All further quantities have to be obtained from the above variables using an equation of state or other closure relations.

Now we study the most important properties of the averaging.

Lemma 1 (Preservation property). *Let $\Psi(t,\cdot) \in L^1(\Omega_L(t))$ and Ψ_α for finitely many bubbles be any extensive variable, then we have*

$$\int_{\Omega_L(t)} \Psi(t,\mathbf{x})\, d\mathbf{x} + \sum_\alpha \Psi_\alpha(t) V_\alpha(t) = \int_{\mathbb{R}^3} (1-c)\overline{\Psi}(t,\mathbf{x}) + c\overline{\Psi_\alpha}(t,\mathbf{x})\, d\mathbf{x}\,.$$

Proof. Using the definitions (4), (2), the Fubini Theorem as well as the fact that $\int_{\mathbb{R}^3} \chi_a \, d\mathbf{x} = 1$ we find

$$
\begin{aligned}
&\int_{\mathbb{R}^3} (1-c)\overline{\Psi}(t,\mathbf{x}) + c\overline{\Psi_\alpha}(t,\mathbf{x}) \, d\mathbf{x} \\
&\qquad = \int_{\mathbb{R}^3} \left[\int_{\Omega_L(t)} \Psi(t,\mathbf{x}') \, \chi_a(\mathbf{x}-\mathbf{x}') \, d\mathbf{x}' + \sum_\alpha \Psi_\alpha(t) \, \chi_a(\mathbf{x}-\mathbf{q}_\alpha(t)) V_\alpha(t) \right] d\mathbf{x} \\
&\qquad = \int_{\Omega_L(t)} \Psi(t,\mathbf{x}') \int_{\mathbb{R}^3} \chi_a(\mathbf{x}-\mathbf{x}') \, d\mathbf{x} \, d\mathbf{x}' + \sum_\alpha \Psi_\alpha(t) \int_{\mathbb{R}^3} \chi_a(\mathbf{x}-\mathbf{q}_\alpha(t)) \, d\mathbf{x} \, V_\alpha(t) \\
&\qquad = \int_{\Omega_L(t)} \Psi(t,\mathbf{x}') \, d\mathbf{x}' + \sum_\alpha \Psi_\alpha(t) V_\alpha(t).
\end{aligned}
$$

□

Next we derive the transport theorems that describe the dynamics of the averaged quantities.

Lemma 2 (Bubble transport equation)**.** *We consider any extensive quantity $\Psi_\alpha(t)$ describing the bubble. We use the notation $\nabla_{\mathbf{x}} = \left(\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \frac{\partial}{\partial x_3}\right)$ for the spatial gradient. Then the averaged quantity $\overline{\Psi_\alpha}$ satisfies the transport equation*

$$
\frac{\partial c\overline{\Psi_\alpha}}{\partial t}(t,\mathbf{x}) + \nabla_{\mathbf{x}} \cdot (c\overline{\Psi_\alpha \dot{\mathbf{q}}_\alpha}(t,\mathbf{x})) = c\overline{\left(\frac{(\Psi_\alpha V_\alpha)^{\cdot}}{V_\alpha}\right)}(t,\mathbf{x}). \tag{12}
$$

Proof. Using the definition (4) we find by differentiation in the sense of distributions, see also Appendix B, and again use of (4)

$$
\begin{aligned}
\frac{\partial}{\partial t} c\overline{\Psi_\alpha}(t,\mathbf{x}) &= \sum_\alpha \frac{\partial}{\partial t}\Big(\Psi_\alpha(t) \, \chi_a(\mathbf{x}-\mathbf{q}_\alpha(t)) V_\alpha(t)\Big) \\
&= \sum_\alpha \Big[\Psi_\alpha(t) \nabla_{\mathbf{q}_\alpha} \chi_a(\mathbf{x}-\mathbf{q}_\alpha(t)) \cdot \dot{\mathbf{q}}_\alpha(t) V_\alpha(t) + \dot{\Psi}_\alpha(t) \, \chi_a(\mathbf{x}-\mathbf{q}_\alpha(t)) V_\alpha(t) \\
&\quad + \Psi_\alpha(t) \, \chi_a(\mathbf{x}-\mathbf{q}_\alpha(t)) \dot{V}_\alpha(t)\Big] \\
&= -\nabla_{\mathbf{x}} \cdot \sum_\alpha \Psi_\alpha(t) \, \chi_a(\mathbf{x}-\mathbf{q}_\alpha(t)) V_\alpha(t) \dot{\mathbf{q}}_\alpha + \sum_\alpha \dot{\Psi}_\alpha(t) \, \chi_a(\mathbf{x}-\mathbf{q}_\alpha(t)) V_\alpha(t) \\
&\quad + \sum_\alpha \Psi_\alpha(t) \frac{\dot{V}_\alpha(t)}{V_\alpha(t)} \chi_a(\mathbf{x}-\mathbf{q}_\alpha(t)) V_\alpha(t) \\
&= -\nabla_{\mathbf{x}} \cdot \big(c\overline{\Psi_\alpha \dot{\mathbf{q}}_\alpha}(t,\mathbf{x})\big) + c\overline{\left(\frac{\dot{\Psi}_\alpha V_\alpha}{V_\alpha}\right)}(t,\mathbf{x}) + c\overline{\left(\frac{\Psi_\alpha \dot{V}_\alpha}{V_\alpha}\right)}(t,\mathbf{x}).
\end{aligned}
$$

□

Note that from the proof we have

$$
c\overline{\dot{\Psi}_\alpha}(t,\mathbf{x}) = \frac{\partial}{\partial t}(c\overline{\Psi_\alpha}(t,\mathbf{x})) + \nabla_{\mathbf{x}} \cdot \big(c\overline{\Psi_\alpha \dot{\mathbf{q}}_\alpha}(t,\mathbf{x})\big) - c\overline{\left(\frac{\Psi_\alpha \dot{V}_\alpha}{V_\alpha}\right)}(t,\mathbf{x}).
$$

Taking $\Psi_\alpha = 1$ in (12) we obtain

$$\frac{\partial c}{\partial t}(t,\mathbf{x}) + \nabla_{\mathbf{x}} \cdot (c\,\overline{\dot{\mathbf{q}}_\alpha}(t,\mathbf{x})) = c\,\overline{\left(\frac{\dot{V}_\alpha}{V_\alpha}\right)}(t,\mathbf{x}). \tag{13}$$

This result states that the volume fraction of the bubbles gets transported by the local average velocity of the balls $\overline{\dot{q}_\alpha}$. According to (13) the volume fraction can also be produced by the source term of the right hand side. This fact indicates that we allow liquid-vapor phase transitions. Note that in Drew and Passman [5] this equation is replaced by the so-called topological equation for the averaged characteristic function of the set microscopically occupied by one phase. But they have not accounted for the phase transition term.

Since we are assuming a spherical shape of V_α note that

$$\frac{\dot{V}_\alpha}{V_\alpha} = 3\frac{\dot{R}_\alpha}{R_\alpha}\,. \tag{14}$$

The next equation of our hierarchy describes the evolution of the number density of bubbles. Taking (6) and $\Psi_\alpha = 1/V_\alpha$ gives

$$\frac{\partial cn}{\partial t}(t,\mathbf{x}) + \nabla_{\mathbf{x}} \cdot (c\,\overline{\dot{\mathbf{q}}_\alpha / V_\alpha}(t,\mathbf{x})) = 0\,. \tag{15}$$

Note that the total number of bubbles in the system does not change. Taking $\Psi_\alpha = \rho_\alpha$ resp. $\Psi_\alpha = \rho_\alpha \dot{q}_\alpha$ we obtain the transport equations for mean bubble mass

$$\frac{\partial c\rho_B}{\partial t}(t,\mathbf{x}) + \nabla_{\mathbf{x}} \cdot (c\rho_B \mathbf{v}_B(t,\mathbf{x})) = c\,\overline{\left(\frac{\dot{m}_\alpha}{V_\alpha}\right)}(t,\mathbf{x}) \tag{16}$$

and mean bubble momentum

$$\frac{\partial c\rho_B v_B}{\partial t}(t,\mathbf{x}) + \nabla_{\mathbf{x}} \cdot (c\,\overline{\rho_\alpha \dot{\mathbf{q}}_\alpha \otimes \dot{\mathbf{q}}_\alpha}(t,\mathbf{x})) = c\,\overline{\left(\frac{(\rho_\alpha \dot{\mathbf{q}}_\alpha V_\alpha)^{\cdot}}{V_\alpha}\right)}(t,\mathbf{x}) = c\,\overline{\left(\frac{(m_\alpha \dot{\mathbf{q}}_\alpha)^{\cdot}}{V_\alpha}\right)}(t,\mathbf{x})\,. \tag{17}$$

Further we obtain with $\Psi_\alpha = \rho_\alpha e_\alpha$ the transport equation for the mean bubble energy

$$\frac{\partial c\rho_B e_B}{\partial t}(t,\mathbf{x}) + \nabla_{\mathbf{x}} \cdot (c\,\overline{\rho_\alpha e_\alpha \dot{\mathbf{q}}_\alpha}(t,\mathbf{x})) = c\,\overline{\left(\frac{(m_\alpha e_\alpha)^{\cdot}}{V_\alpha}\right)}(t,\mathbf{x})\,. \tag{18}$$

In order to obtain the corresponding transport equations for the liquid phase we will need differentiation in time of integrals with time dependent integrand and domain of integration of the form

$$\frac{d}{dt}\int_{\Omega(t)} \Psi(t,y)\,dy.$$

This is achieved by the well known Reynolds Transport Theorem assuming that we know a continuously differentiable family of continuously differentiable transformations $\mathbf{X}^t : \Omega(0) \to \Omega(t)$ whereby for each point y_0 we have a trajectory $y(t) = \mathbf{X}^t(y_0)$ leading to a velocity field $\mathbf{u}(t,y) = \dot{y}(t)$.

Theorem 1 (Reynolds Transport Theorem)**.** *Let $\Psi : \mathbb{R} \times \mathbb{R}^{\mathsf{N}} \to \mathbb{R}$ be a continuously differentiable scalar field and the transformations $\mathbf{X}^t : \mathbb{R}^{\mathsf{N}} \to \mathbb{R}^{\mathsf{N}}$ also continuously differentiable with the velocity field $\mathbf{u}$ as defined above. Then for any bounded control volume $\Omega(t)$ the transport equation*

$$\frac{d}{dt}\int_{\Omega(t)} \Psi(t,y)\,dy = \int_{\Omega(t)} \left[\frac{\partial \Psi}{\partial t}(t,y) + \nabla_y \cdot \Big(\Psi(t,y)\mathbf{u}(t,y)\Big)\right] dy \tag{19}$$

holds, where $\boldsymbol{\eta}(t)$ is the velocity of the boundary.

Proof. A proof can be found in Serrin [18] or Warnecke [21]. □

Also see Drew and Passman [5, p. 102] for the topological equation. For our purposes we will modify the equation (19) using the Gauss theorem with the outer unit normal field $\boldsymbol{\eta}(t)$ on the boundary $\partial\Omega(t)$ giving

$$\frac{d}{dt}\int_{\Omega(t)} \Psi(t,y)\,dy = \int_{\Omega(t)} \frac{\partial \Psi}{\partial t}(t,y)\,dy + \oint_{\partial\Omega(t)} \Big(\Psi(t,y)\mathbf{u}(t,y)\Big)\cdot \boldsymbol{\eta}(t,y)\,dS. \tag{20}$$

Lemma 3 (General transport equation)**.** *Let us assume that a physical quantity Ψ for the carrier fluid satisfies a microscopic balance law*

$$\frac{\partial}{\partial t}\Psi(t,\mathbf{x}') + \nabla_{\mathbf{x}'} \cdot \mathbf{F}(t,\mathbf{x}') = G(t,\mathbf{x}') \tag{21}$$

for some given flux function $\mathbf{F}$ and right hand side G, e.g. an external force or a source. We set $I_\alpha(t) = \partial B_\alpha(t)$ and take $\boldsymbol{\eta}_\alpha$ to be the outer unit normal vector of these balls on their surface. We further denote by $\mathbf{R}_\alpha(t) = R_\alpha(t)\boldsymbol{\eta}_\alpha$ the vector of length $R_\alpha(t)$ so that $\mathbf{q}_\alpha(t) + \mathbf{R}_\alpha(t)$ gives an arbitrary point on $\partial B_\alpha(t)$. We set $\mathbf{w}_\alpha = \dot{\mathbf{q}}_\alpha + \dot{\mathbf{R}}_\alpha$. Further, we assume that the boundary ∂ of the ball $B_a(\mathbf{x})$ does not intersect any of the small balls $B_\alpha(t)$. Then we have by averaging nn

$$\begin{aligned}\frac{\partial}{\partial t}&(1-c)\overline{\Psi}(t,\mathbf{x}) + \nabla_{\mathbf{x}} \cdot (1-c)\overline{\mathbf{F}}(t,\mathbf{x}) \\ &= \sum_{\substack{\alpha \\ \mathbf{q}_\alpha \in B_a(\mathbf{x})}} \oint_{I_\alpha(t)} \big[\mathbf{F}(t,\mathbf{x}') - \Psi(t,\mathbf{x}')\mathbf{w}_\alpha\big]\cdot \boldsymbol{\eta}_\alpha\, \chi_a(\mathbf{x}-\mathbf{x}')\,dS + (1-c)\overline{G}(t,\mathbf{x}).\end{aligned} \tag{22}$$

The summation is finite and by assumption the quantities $\dot{\mathbf{q}}_\alpha$, $\dot{\mathbf{R}}_\alpha$ are constant with respect to integration on each sphere.

Proof. We have to take into account that our general averaging integral in (2) has a time dependent domain of integration and use (20). The unit normals $\boldsymbol{\eta}_\alpha$ are inner unit normals to $\Omega_{L(t)}$, so we obtain

$$\begin{aligned}\frac{\partial}{\partial t}(1-c)\overline{\Psi}(t,\mathbf{x}) &= \frac{\partial}{\partial t}\int_{\Omega_{L(t)}} \Psi(t,\mathbf{x}')\,\chi_a(\mathbf{x}-\mathbf{x}')\,d\mathbf{x}' \\ &= \int_{\Omega_{L(t)}} \frac{\partial \Psi}{\partial t}(t,\mathbf{x}')\,\chi_a(\mathbf{x}-\mathbf{x}')\,d\mathbf{x}' - \sum_{\alpha} \oint_{I_\alpha(t)} \Psi(t,\mathbf{x}')\mathbf{w}_\alpha \cdot \boldsymbol{\eta}_\alpha(t)\,\chi_a(\mathbf{x}-\mathbf{x}')\,dS.\end{aligned} \tag{23}$$

The summation is taken over all balls with their center in the support of $\chi_a(\mathbf{x}-\mathbf{x}')$. Now we use the conservation law (21) and (2) as well as the shift of differentiation formula for the distribution $\nabla_{\mathbf{x}'}\chi_a(\mathbf{x}-\mathbf{x}')$ given in Appendix B to obtain

$$\begin{aligned}
\frac{\partial}{\partial t}(1-c)\overline{\Psi}(t,\mathbf{x}) =& -\int_{\Omega_{L(t)}} \nabla_{\mathbf{x}'}\cdot\mathbf{F}(t,\mathbf{x}')\,\chi_a(\mathbf{x}-\mathbf{x}')\,d\mathbf{x}' + \int_{\Omega_{L(t)}} G(t,\mathbf{x}')\,\chi_a(\mathbf{x}-\mathbf{x}')\,d\mathbf{x}' \\
&-\sum_\alpha \oint_{I_\alpha(t)} \Psi(t,\mathbf{x}')\mathbf{w}_\alpha\cdot\boldsymbol{\eta}_\alpha(t)\,\chi_a(\mathbf{x}-\mathbf{x}')\,dS \\
=& -\int_{\Omega_{L(t)}} \nabla_{\mathbf{x}'}\cdot\left[\mathbf{F}(t,\mathbf{x}')\,\chi_a(\mathbf{x}-\mathbf{x}')\right]d\mathbf{x}' + \int_{\Omega_{L(t)}} \mathbf{F}(t,\mathbf{x}')\nabla_{\mathbf{x}'}\chi_a(\mathbf{x}-\mathbf{x}')\,d\mathbf{x}' \\
&-\sum_\alpha \oint_{I_\alpha(t)} \Psi(t,\mathbf{x}')\mathbf{w}_\alpha\cdot\boldsymbol{\eta}_\alpha(t)\,\chi_a(\mathbf{x}-\mathbf{x}')\,dS + (1-c)\overline{G}(t,\mathbf{x}).
\end{aligned}$$

Using the shift of differentiation formula from Appendix B this gives

$$\begin{aligned}
\frac{\partial}{\partial t}(1-c)\overline{\Psi}(t,\mathbf{x}) =& -\int_{\Omega_{L(t)}} \nabla_{\mathbf{x}'}\cdot\left[\mathbf{F}(t,\mathbf{x}')\,\chi_a(\mathbf{x}-\mathbf{x}')\right]d\mathbf{x}' - \nabla_{\mathbf{x}}\cdot\int_{\Omega_{L(t)}} \mathbf{F}(t,\mathbf{x}')\,\chi_a(\mathbf{x}-\mathbf{x}')\,d\mathbf{x}' \\
&-\sum_\alpha \oint_{I_\alpha(t)} \Psi(t,\mathbf{x}')\mathbf{w}_\alpha\cdot\boldsymbol{\eta}_\alpha(t)\,\chi_a(\mathbf{x}-\mathbf{x}')\,dS + (1-c)\overline{G}(t,\mathbf{x}) \\
=& \sum_\alpha \oint_{I_\alpha(t)} \mathbf{F}(t,\mathbf{x}')\cdot\boldsymbol{\eta}_\alpha(t,\mathbf{x}')\,\chi_a(\mathbf{x}-\mathbf{x}')\,dS - \nabla_{\mathbf{x}}\cdot(1-c)\overline{\mathbf{F}}(t,\mathbf{x}) \\
&-\sum_\alpha \oint_{I_\alpha(t)} \Psi(t,\mathbf{x}')\mathbf{w}_\alpha\cdot\boldsymbol{\eta}_\alpha(t)\,\chi_a(\mathbf{x}-\mathbf{x}')\,dS + (1-c)\overline{G}(t,\mathbf{x}).
\end{aligned}$$

All terms involving derivatives of χ_a have to be interpreted in the sense of distributions, see Appendix B. $\square$

For the case that small balls $B_\alpha(t)$ intersect $\partial B_a(\mathbf{x})$ we take the same formula (22) and again make a small error, as in the definition of c.

For a first illustration we consider the special case $\Psi = 1$ to obtain an equation for the concentration c in the liquid setting. We have

$$\begin{aligned}
\frac{\partial}{\partial t}(1-c)(t,\mathbf{x}) =& -\frac{\partial c}{\partial t}(t,\mathbf{x}) = -\frac{\partial}{\partial t}\int_{\Omega_{L(t)}} \chi_a(\mathbf{x}-\mathbf{x}')\,d\mathbf{x}' \\
=& -\sum_\alpha \oint_{I_\alpha(t)} \mathbf{w}_\alpha\cdot\boldsymbol{\eta}_\alpha(t)\,\chi_a(\mathbf{x}-\mathbf{x}')\,dS \\
=& -\sum_\alpha \oint_{I_\alpha(t)} \left(\dot{\mathbf{q}}_\alpha + \dot{\mathbf{R}}_\alpha\right)\cdot\boldsymbol{\eta}_\alpha(t)\,\chi_a(\mathbf{x}-\mathbf{x}')\,dS \\
=& -\sum_\alpha \int_{B_\alpha(t)} \nabla_{\mathbf{x}'}\cdot\left[\dot{\mathbf{q}}_\alpha\,\chi_a(\mathbf{x}-\mathbf{x}')\right]d\mathbf{x}' - \sum_\alpha \oint_{I_\alpha(t)} \dot{R}_\alpha\,\chi_a(\mathbf{x}-\mathbf{x}')\,dS. \\
=& \nabla_x\cdot\sum_\alpha \int_{B_\alpha(t)} \left[\dot{\mathbf{q}}_\alpha\,\chi_a(\mathbf{x}-\mathbf{x}')\right]d\mathbf{x}' - \sum_\alpha \oint_{I_\alpha(t)} \dot{R}_\alpha\,\chi_a(\mathbf{x}-\mathbf{x}')\,dS.
\end{aligned}$$

Now we may set $\chi_a(\mathbf{x}-\mathbf{q}_\alpha(t)) = \chi_a(\mathbf{x}-\mathbf{x}')$, because we note that in case $a > 2R_\alpha(t)$ for all α, which we assume throughout, we have $B_\alpha(t) \subset B_a(\mathbf{q}_\alpha(t)+\mathbf{R}_\alpha(t))$. So for $\mathbf{x} \in B_a(\mathbf{q}_\alpha(t)) \cap B_a(\mathbf{q}_\alpha(t)+\mathbf{R}_\alpha(t))$ we have using $\mathbf{x}' = \mathbf{q}_\alpha(t)+\mathbf{R}_\alpha(t) \in I_\alpha(t)$

$$\chi_a(\mathbf{x}-\mathbf{q}_\alpha(t)) = \chi_a(\mathbf{x}-(\mathbf{q}_\alpha(t)+\mathbf{R}_\alpha(t)) = \chi_a(\mathbf{x}-\mathbf{x}') = \frac{1}{V_a}. \tag{24}$$

This gives

$$\frac{\partial c}{\partial t}(t,\mathbf{x}) + \nabla_{\mathbf{x}} \cdot \left(c(t,\mathbf{x})\overline{\dot{\mathbf{q}}_\alpha}(t,\mathbf{x})\right) = 3c\overline{\left(\frac{\dot{R}}{R}\right)}.$$

Here we refer the reader to the corresponding equations (13) and (14) for the concentration in the bubble setting, which gives the same result.

3 Mixture balance laws

3.1 The microscopic conservation laws within each phase

The liquid is assumed to be described by the inviscid, compressible balances for mass, momentum and energy for the microscopic variables mass density $\rho : \mathbb{R}\times\mathbb{R}^3 \to \mathbb{R}$, velocity $\mathbf{v} : \mathbb{R}\times\mathbb{R}^3 \to \mathbb{R}^3$ and energy $e : \mathbb{R}\times\mathbb{R}^3 \to \mathbb{R}$.

$$\frac{\partial \rho}{\partial t} + \nabla_{\mathbf{x}} \cdot (\rho\,\mathbf{v}) = 0, \tag{25}$$

$$\frac{\partial(\rho\mathbf{v})}{\partial t} + \nabla_{\mathbf{x}}((\rho\mathbf{v}\otimes\mathbf{v}) + p(\rho)\mathbf{1}) = \rho\mathbf{g}, \tag{26}$$

$$\frac{\partial \rho e}{\partial t} + \nabla_{\mathbf{x}} \cdot ((\rho e + p)\mathbf{v} + \mathbf{Q}) = \rho\mathbf{g}\cdot\mathbf{v}. \tag{27}$$

The pressure $p : \mathbb{R}\times\mathbb{R}^3 \to \mathbb{R}$ is given by the equation of state due to Hooke's law applied to an isotropic liquid

$$p = p_{ref} + K(\frac{\rho}{\rho_{ref}} - 1), \tag{28}$$

where K is the liquid bulk modulus. This means, that the liquid density does not depend on temperature, we neglect thermal expansion. Corresponding to equation (28) the speed of sound a_L of the liquid is given by

$$a_L = \sqrt{\frac{K}{\rho_{ref}}} \tag{29}$$

and is obviously constant. The gravitational acceleration is given by $\mathbf{g} = -g(0,0,1)$. For the energy we have

$$e = u + \frac{1}{2}\mathbf{v}^2,$$

where we use the following constitutive law for the internal energy u

$$u(T,\rho) = c_*(T - T_{ref}) + (p_{ref} - K)\left(\frac{1}{\rho_{ref}} - \frac{1}{\rho}\right) + \frac{K}{\rho_{ref}}\ln\frac{\rho}{\rho_{ref}} + u(T_{ref},\rho_{ref}) \tag{30}$$

with the specific heat capacity c_*. Further we have Fourier's law the constitutive law for the heat flux

$$\mathbf{Q} = -\kappa \nabla T$$

with the heat conductivity κ.

We assume that the content of the bubbles behaves as an ideal gas. It is described by the ideal thermal and the caloric equation of state for the pressure and the internal energy

$$p_\alpha = \frac{\rho_\alpha k T_\alpha}{m_0} \qquad \text{and} \qquad u_\alpha(T_\alpha) = z\frac{k}{m_0}(T_\alpha - T_{ref}) + u(T_{ref}) \tag{31}$$

where m_0 is the molecular mass, k is the Boltzmann constant and $z = 3$ for a polyatomic gas.

The thermodynamic states inside the bubbles are assumed to be homogeneous in space. For this reason we do not need local balance laws here. Instead we take Newton's law of motion for the evolution of the bubble centers $\mathbf{q}_\alpha$, which concerns a moving bubble with changing bubble radius that may gain or lose mass

$$(m_\alpha(t)\dot{q}^j_\alpha(t))^{\cdot} = -\oint_{I_\alpha} p\eta^j_\alpha dS + m_\alpha g^j + \frac{\dot{m}_\alpha(t)}{4\pi R_\alpha(t)^2}\oint_{I_\alpha} v^j(t,\mathbf{x}')dS\,, \tag{32}$$

for $j = 1,2,3$. The first term on the right hand side is the pressure exerted by the fluid onto the particle, the second is the gravitational force and the third term is a momentum change due to mass being lost to the carrier fluid. The special form of these equations is explained in Appendix A.

Further, we have the respective mass, momentum, and energy balance at the interface

$$[\![\rho(v^\eta - w^\eta)]\!] = 0, \tag{33}$$

$$\rho(v^\eta - w^\eta)[\![\mathbf{v}]\!] + [\![p\eta]\!] = 2\sigma k_m \eta\,, \tag{34}$$

$$\rho(v^\eta - w^\eta)[\![u + \frac{p}{\rho} + \frac{1}{2}(\mathbf{v}-\mathbf{w})^2]\!] + [\![Q]\!] = 0, \tag{35}$$

where the jump brackets denote $[\![\Psi]\!] = \Psi^I_L - \Psi^I_\alpha$ for any physical quantity Ψ, σ denotes the surface tension and k_m denotes the mean curvature.

For a simplified study one can ignore the energy equation. In that case one has to introduce a rule that controls the variation of temperature. For instance we can consider either the isothermal or the adiabatic case. In this paper for simplicity we only investigate the isothermal system mathematically, see Section 5. Moreover we illustrate how to deal with source terms resp. evolution laws for the isothermal system, see Section 6 and Section 7.

3.2 Macroscopic mass balances

We first use for the liquid phase (22) with $\Psi = \rho$, $\mathbf{F} = \rho\mathbf{v}$ and the definition (10) to obtain from (25)

$$\frac{\partial}{\partial t}[(1-c)\rho_L](t,\mathbf{x}) + \nabla_{\mathbf{x}}\cdot[(1-c)\rho_L\mathbf{v}_L](t,\mathbf{x}) = \sum_\alpha \oint_{I_\alpha(t)} \rho(t,\mathbf{x}')\left[\mathbf{v}(t,\mathbf{x}') - \mathbf{w}_\alpha(t)\right]\cdot\boldsymbol{\eta}_\alpha\, \chi_a(\mathbf{x}-\mathbf{x}')\, dS\,. \tag{36}$$

For the bubbles we take (12) with $\Psi_\alpha(t) = m_\alpha(t)/V_\alpha(t)$, the definitions (7) and obtain

$$\frac{\partial(c\rho_B)}{\partial t}(t,\mathbf{x}) + \nabla_\mathbf{x}\cdot(c\,\rho_B\mathbf{v}_B)(t,\mathbf{x}) = c\,\overline{\left(\frac{\dot{m}_\alpha}{V_\alpha}\right)}(t,\mathbf{x}). \tag{37}$$

Overall the total mass of both phases must be conserved. Therefore, we must have a mass balance across the interfaces. The terms on the right hand side must cancel when both equations are added together. In fact this happens because we conclude: For $\mathbf{x}' = \mathbf{q}_\alpha(t) + \mathbf{R}_\alpha(t) \in I_\alpha(t)$ we have using (24) for the right hand side of (37)

$$c\,\overline{\left(\frac{\dot{m}_\alpha}{V_\alpha}\right)}(t,\mathbf{x}) = \sum_\alpha \dot{m}_\alpha\, \chi_a(\mathbf{x} - (\mathbf{q}_\alpha(t) + \mathbf{R}_\alpha(t)) = \sum_\alpha \dot{m}_\alpha\, \chi_a(\mathbf{x} - \mathbf{x}')\,.$$

Now for $\mathbf{x}' \in \partial B_\alpha(t)$ and $\mathbf{x} \in B_a(\mathbf{q}_\alpha(t)) \cap B_a(\mathbf{q}_\alpha(t) + \mathbf{R}_\alpha(t))$ we obtain the relation

$$\oint_{I_\alpha(t)} \rho(t,\mathbf{x}')\left[\mathbf{v}(t,\mathbf{x}') - \mathbf{w}_\alpha(t)\right]\cdot\boldsymbol{\eta}_\alpha\, \chi_a(\mathbf{x}-\mathbf{x}')\, dS = -\dot{m}_\alpha\, \chi_a(\mathbf{x}-\mathbf{x}')$$

for the liquid phase. This equation relates the rate of mass change $\dot{m}_\alpha$ to the flow and boundary velocities. We use the rate of mass change

$$\dot{m}_\alpha = -\oint_{I_\alpha(t)} \rho(t,\mathbf{x}')\left[\mathbf{v}(t,\mathbf{x}') - \mathbf{w}_\alpha(t)\right]\cdot\boldsymbol{\eta}_\alpha\, dS\,. \tag{38}$$

The total rate of change of mass in $B_\alpha(t)$ equals the mass flux at the moving fluid boundary. A change of bubble mass corresponds to a positive (gain) resp. negative (loss) boundary velocity $w_\alpha = \mathbf{w}_\alpha\cdot\boldsymbol{\eta}_\alpha = (\dot{\mathbf{q}}_\alpha + \dot{\mathbf{R}}_\alpha)\cdot\boldsymbol{\eta}_\alpha$.

Therefore, summation over α gives identical right hand sides of equations (36) and (37), i.e. total mass conservation.

3.3 Macroscopic momentum balances

For the liquid phase we use (22) with $\Psi = \rho\mathbf{v}$, $\mathbf{F} = \rho\mathbf{v}\otimes\mathbf{v} + p\mathbf{1}$, set $G = \rho\mathbf{g}$ and take p given by the equation of state (28) to obtain

$$\begin{aligned}
\frac{\partial}{\partial t}&[(1-c)\rho_L\mathbf{v}_L](t,\mathbf{x}) + \nabla_\mathbf{x}\cdot([(1-c)\overline{\rho\mathbf{v}\otimes\mathbf{v}}](t,\mathbf{x}) + (1-c)p_L\mathbf{1}) - (1-c)\rho_L\mathbf{g} \\
&= \sum_\alpha \oint_{I_\alpha(t)} \left[\rho\mathbf{v}(t,\mathbf{x}')\otimes[\mathbf{v}(t,\mathbf{x}') - \mathbf{w}_\alpha] + p(t,\mathbf{x}')\mathbf{1}\right]\cdot\boldsymbol{\eta}_\alpha\, \chi_a(\mathbf{x}-\mathbf{x}')\, dS \\
&= \sum_\alpha \left(\oint_{I_\alpha(t)} \rho\mathbf{v}(t,\mathbf{x}')\otimes[\mathbf{v}(t,\mathbf{x}') - \mathbf{w}_\alpha]\cdot\boldsymbol{\eta}_\alpha\, \chi_a(\mathbf{x}-\mathbf{x}')\, dS \right. \\
&\quad \left. + \oint_{I_\alpha(t)} p(t,\mathbf{x}')\boldsymbol{\eta}_\alpha\, \chi_a(\mathbf{x}-\mathbf{x}')\, dS\right).
\end{aligned} \tag{39}$$

For the disperse phase we now take (12) with $\mathbf{\Psi}_\alpha(t) = \rho_\alpha(t)\dot{\mathbf{q}}_\alpha(t)$. This gives

$$\frac{\partial(c\rho_B\mathbf{v}_B)}{\partial t}(t,\mathbf{x}) + \nabla_\mathbf{x}\cdot(c\overline{\rho_\alpha\dot{\mathbf{q}}_\alpha\otimes\dot{\mathbf{q}}_\alpha})(t,\mathbf{x}) = c\overline{\left(\frac{(\rho_\alpha\dot{\mathbf{q}}_\alpha V_\alpha)^{\cdot}}{V_\alpha}\right)}(t,\mathbf{x}) = c\overline{\left(\frac{(m_\alpha\dot{\mathbf{q}}_\alpha)^{\cdot}}{V_\alpha}\right)}(t,\mathbf{x}).$$

Now we may consider (32) on the right hand side. We obtain using (4)

$$\begin{aligned} c\overline{\left(\frac{(m_\alpha\dot{\mathbf{q}}_\alpha)^{\cdot}}{V_\alpha}\right)}(t,\mathbf{x}) &= -c\overline{\left(\oint_{I_\alpha} p\boldsymbol{\eta}_\alpha dS/V_\alpha\right)} + c\overline{\left(\frac{m_\alpha}{V_\alpha}\right)}\mathbf{g} + c\overline{\left(\frac{\dot{m}_\alpha(t)}{4\pi R_\alpha(t)^2}\oint_{I_\alpha}\mathbf{v}dS/V_\alpha\right)} \\ &= \sum_\alpha\left(-\oint_{I_\alpha} p\boldsymbol{\eta}_\alpha dS + \frac{\dot{m}_\alpha(t)}{4\pi R_\alpha(t)^2}\oint_{I_\alpha}\mathbf{v}dS\right)\chi_a(\mathbf{x}-\mathbf{q}_\alpha(t)) + c\rho_B\mathbf{g}. \end{aligned} \tag{40}$$

Again the momenta must balance across the interfaces. In analogy to the above arguments for the mass balance, we obtain the momentum balance on the interfaces

$$\begin{aligned} &\oint_{I_\alpha} p\eta_\alpha^j dS - \frac{\dot{m}_\alpha(t)}{4\pi R_\alpha(t)^2}\oint_{I_\alpha} v^j dS \\ &\qquad = \oint_{I_\alpha}\rho v^j[\mathbf{v}-\mathbf{w}_\alpha]\cdot\boldsymbol{\eta}_\alpha\, dS + \oint_{I_\alpha} p\eta_\alpha^j\, dS\,. \end{aligned}$$

This equation obviously holds, because of the mass balance at the interface

$$-\frac{\dot{m}_\alpha(t)}{4\pi R_\alpha(t)^2}\oint_{I_\alpha} v^j dS = \oint_{I_\alpha}\rho v^j[\mathbf{v}-\mathbf{w}_\alpha]\cdot\boldsymbol{\eta}_\alpha\, dS\,. \tag{41}$$

3.4 Macroscopic energy balances

To obtain an energy balance equation for the liquid phase, we again use (22) with $\Psi = \rho e$, $\mathbf{F} = (\rho e + p)\mathbf{v} + \mathbf{Q}$ and $G = \rho\mathbf{g}\cdot\mathbf{v}$. We get

$$\begin{aligned} \frac{\partial}{\partial t}(1-c)\rho_L e_L \quad &+ \quad \nabla_x\cdot(1-c)\overline{(\rho e+p)\mathbf{v}+\mathbf{Q}} - (1-c)\rho_L\mathbf{g}\cdot\mathbf{v}_L \\ &= \quad \sum_\alpha\oint_{I_\alpha}((\rho e+p)\mathbf{v}-\rho e\mathbf{w}+\mathbf{Q})\cdot\eta\chi_a(\mathbf{x}-\mathbf{q}_\alpha)\,dS \\ &= \quad \sum_\alpha\oint_{I_\alpha}(\rho(\mathbf{v}-\mathbf{w})e+p\mathbf{v}+\mathbf{Q})\cdot\eta\chi_a(\mathbf{x}-\mathbf{q}_\alpha)\,dS \end{aligned} \tag{42}$$

Again we take for the disperse phase (12) with $\Psi_\alpha(t) = \rho_\alpha(t)e_\alpha(t)$ to obtain

$$\frac{\partial c\rho_B e_B}{\partial t} + \nabla_\mathbf{x}\cdot(c\overline{\rho_\alpha e_\alpha\dot{\mathbf{q}}_\alpha})(t,\mathbf{x}) = c\overline{\left(\frac{(m_\alpha e_\alpha)^{\cdot}}{V_\alpha}\right)}(t,\mathbf{x})\,. \tag{43}$$

For the right hand side of (43) we have

$$c\overline{\left(\frac{(m_\alpha e_\alpha)^{\cdot}}{V_\alpha}\right)}(t,\mathbf{x}) + c\rho_B\mathbf{g}\cdot\mathbf{v}_B = -\sum_\alpha\oint_{I_\alpha}(\rho(\mathbf{v}-\mathbf{w})e+p\mathbf{v}+\mathbf{Q})\cdot\eta\chi_a(\mathbf{x}-\mathbf{q}_\alpha)\,dS\,.$$

This implies energy conservation at the interface.

4 Closure relations

The PDE system, we are interested in, relies on the balance equations that were derived in the last section. In these equations several quantities appear that must be related to the variables of the model, namely

$$\overline{\left(\frac{\dot{\mathbf{q}}_\alpha}{V_\alpha}\right)}, \quad \overline{\left(\frac{\dot{R}_\alpha}{R_\alpha}\right)}, \quad \overline{\left(\frac{\dot{m}_\alpha}{V_\alpha}\right)}, \quad \overline{\rho_\alpha(t)\dot{\mathbf{q}}_\alpha \otimes \dot{\mathbf{q}}_\alpha}, \quad \overline{\frac{1}{V_\alpha}\oint_{I_\alpha} p\eta^j_\alpha dS}, \quad \overline{(\rho e + p)\mathbf{v} + \mathbf{Q}},$$

$$\overline{\left(\frac{\dot{m}_\alpha(t)}{4\pi R_\alpha(t)^2}\oint_{I_\alpha} v^j dS/V_\alpha\right)}, \quad \overline{\rho\mathbf{v}\otimes\mathbf{v}}, \quad \overline{\rho_\alpha e_\alpha \dot{\mathbf{q}}_\alpha}, \quad \overline{\frac{1}{V_\alpha}\oint(\rho(\mathbf{v}-\mathbf{w})e + p\mathbf{v} + \mathbf{Q})\cdot\eta\, ds}.$$

Now we will modify these expressions in order to obtain a closed system of equations. At first we introduce the *cold closure assumption* to simplify the first and fourth term. To this end we decompose the bubble velocity $\dot{\mathbf{q}}_\alpha$ as $\dot{\mathbf{q}}_\alpha = \mathbf{v}_B + \mathbf{C}_\alpha$. The cold closure assumption ignores the excess velocity $\mathbf{C}_\alpha$, this means we ignore any stochastic motion of the bubbles. Using (6) and (5) this assumption leads to

$$\overline{\left(\frac{\dot{\mathbf{q}}_\alpha}{V_\alpha}\right)} = n\mathbf{v}_B \qquad \text{and} \qquad \overline{\rho_\alpha(t)\dot{\mathbf{q}}_\alpha \otimes \dot{\mathbf{q}}_\alpha} = \rho_B \mathbf{v}_B \otimes \mathbf{v}_B\,. \tag{44}$$

Alternatively one could introduce a Reynolds stress tensor. This requires additional modeling in order to close the system. It is no easy task, see e.g. Drew and Passman [5].

Similarly we set

$$\overline{\rho\mathbf{v}\otimes\mathbf{v}} = \rho_L \mathbf{v}_L \otimes \mathbf{v}_L \quad , \quad \overline{\rho_\alpha e_\alpha \dot{\mathbf{q}}_\alpha} = \rho_B \mathbf{v}_B e_B \quad \text{and} \quad \overline{(\rho e + p)\mathbf{v}} = (\rho_L e_L + p_L)\mathbf{v}_L$$

and define the averaged bubble resp. liquid internal energy

$$u_B := e_B - \frac{1}{2}\mathbf{v}_B^2 \qquad \text{and} \qquad u_L := e_L - \frac{1}{2}\mathbf{v}_L^2\,.$$

Further we define the averaged temperatures of the phases

$$T_B := (u_B - u_{ref}(T_{ref}))\frac{m_0}{zk} + T_{ref} \qquad \text{and}$$

$$T_L := \frac{1}{c_*}\left(u_L - u_{ref}(T_{ref},\rho_{ref}) - (p_{ref} - K)\left(\frac{1}{\rho_{ref}} - \frac{1}{\rho_L}\right) - \frac{K}{\rho_{ref}}\ln\frac{\rho}{\rho_{ref}}\right) + T_{ref}$$

with the same reference data as in (30) and (31). With this definition we set

$$\overline{\mathbf{Q}} = -\kappa\nabla T_L\,.$$

Next we calculate the second and third expression of our list. At first we have by definition

$$c\overline{\left(\frac{\dot{R}_\alpha}{R_\alpha}\right)}(t,\mathbf{x}) = \sum_\alpha \frac{\dot{R}_\alpha(t)}{R_\alpha(t)}\chi_\alpha(\mathbf{x}-\mathbf{q}_\alpha(t))V_\alpha(t)\,, \; c\overline{\left(\frac{\dot{m}_\alpha}{V_\alpha}\right)}(t,\mathbf{x}) = \sum_\alpha \dot{m}_\alpha(t)\chi_\alpha(\mathbf{x}-\mathbf{q}_\alpha(t))\,.$$

The evolution of $R_\alpha(t)$ and $m_\alpha(t)$ was studied in [4] for a single bubble. There we considered various model equations without and with phase transition. These equations are used here to determine $\dot{R} = \overline{\dot{R}_\alpha}$ and $\dot{m} = \overline{\dot{m}_\alpha}$ by the simplifying assumption that we set

$$\overline{\left(\frac{\dot{R}_\alpha}{R_\alpha}\right)} = \frac{\dot{R}}{R} \quad \text{and} \quad \overline{\left(\frac{\dot{m}_\alpha}{V_\alpha}\right)} = \frac{\dot{m}}{V}, \tag{45}$$

where R and V denote the mean bubble radius resp. the mean bubble volume. These quantities are related to the volume fraction c and the number density cn. We have

$$\frac{c}{cn} = \frac{1}{n} = V = \frac{4\pi R^3}{3}. \tag{46}$$

The right hand sides of (45) are calculated by means of the models from [4], see Section 6 for more details.

Further, we now replace the fifth term and the seventh term of the list. We use equation (41) and the interfacial momentum balance equation (34). For the spherical bubble with index α the mean curvature is given by $-1/R_\alpha$. Therefore we have

$$\begin{aligned}
\oint_{I_\alpha} \left(\rho v^j [\mathbf{v} - \mathbf{w}_\alpha] \cdot \boldsymbol{\eta}_\alpha + p\eta_\alpha^j\right) dS &= \oint_{I_\alpha} \left(\rho_\alpha v_\alpha^j [\mathbf{v}_\alpha - \mathbf{w}_\alpha] \cdot \boldsymbol{\eta}_\alpha + (p_\alpha - \frac{2\sigma}{R_\alpha})\eta_\alpha^j\right) dS \\
&= -\frac{\dot{m}_\alpha}{4\pi R_\alpha^2} \oint v_\alpha^j \, dS = -\frac{\dot{m}_\alpha}{4\pi R_\alpha^2} \oint \dot{q}_\alpha^j \, dS \\
&= -\dot{m}_\alpha \dot{q}_\alpha^j.
\end{aligned} \tag{47}$$

This expression is zero in the radially symmetric case of a single spherical bubble.

In order to modify the last expression of the list, we use the interface balances for energy (35) and momentum (34) as well as the mass balance at the interface (33) to obtain

$$\begin{aligned}
\frac{1}{V_\alpha} \oint (\rho(\mathbf{v} - \mathbf{w})e &+ p\mathbf{v} + \mathbf{Q}) \cdot \eta \, ds = \frac{1}{V_\alpha} \oint (\rho_\alpha(\mathbf{v}_\alpha - \mathbf{w})e_\alpha + p_\alpha \mathbf{v}_\alpha + \mathbf{Q}_\alpha + 2\sigma k_m \mathbf{w}) \cdot \eta \, ds \\
&= -\frac{\dot{m}_\alpha e_\alpha}{V_\alpha} - \frac{p_\alpha \dot{m}_\alpha}{\rho_\alpha V_\alpha} + \frac{3p_\alpha \dot{R}_\alpha}{R_\alpha} - \frac{6\sigma \dot{R}_\alpha}{R_\alpha^2} + \frac{1}{V_\alpha} \oint \mathbf{Q}_\alpha \cdot \eta \, ds
\end{aligned}$$

with

$$\frac{1}{V_\alpha} \oint \mathbf{Q}_\alpha \cdot \eta \, ds = \frac{3Q_\alpha^I}{R_\alpha}.$$

Integrating the energy balance equation for a radial symmetric homogeneous bubble

$$r^2 p_\alpha \frac{\partial}{\partial t} \ln \frac{T_\alpha^z}{\rho_\alpha} + \frac{\partial r^2 Q_\alpha}{\partial r} = 0$$

over the whole bubble domain we obtain

$$\frac{3Q_\alpha^I}{R_\alpha} = -\rho_\alpha \dot{T}_\alpha \frac{kz}{m_0} + \frac{p_\alpha \dot{m}_\alpha}{\rho_\alpha V_\alpha} - \frac{3p_\alpha \dot{R}_\alpha}{R_\alpha}.$$

As above, we set $\overline{\Pi}_m = \Pi_m$ with

$$\Pi_m^j = -c\frac{\dot{m}v_B^j}{\frac{4}{3}\pi R^3}\,. \tag{48}$$

Similarly, we define

$$\Pi_c = 3c\frac{\dot{R}}{R} \qquad , \qquad \Pi_\rho = c\frac{\dot{m}}{\frac{4}{3}\pi R^3} \qquad \text{and} \qquad \Pi_e = c\frac{\dot{m}e_B}{\frac{4}{3}\pi R^3} + c\rho_B\dot{T}\frac{kz}{m_0} + 6c\frac{\sigma\dot{R}}{R^2}\,. \tag{49}$$

Thus we end up with 8 partial differential equations for the determination of the variables number density n, volume fraction of the disperse phase c, densities of the phases ρ_L, ρ_B, velocities of the phases $\mathbf{v}_L$, $\mathbf{v}_B$ and energy of the phases e_L, e_B. In summary the system of partial differential equations can be written as

$$\begin{aligned}
\frac{\partial cn}{\partial t} + \nabla_{\mathbf{x}}\cdot(cn\mathbf{v}_B) &= 0\,,\\
\frac{\partial c}{\partial t} + \nabla_{\mathbf{x}}\cdot(c\mathbf{v}_B) &= \Pi_c\,,\\
\frac{\partial}{\partial t}[(1-c)\rho_L] + \nabla_{\mathbf{x}}\cdot[(1-c)\rho_L\mathbf{v}_L] &= -\,\Pi_\rho\,,\\
\frac{\partial c\rho_B}{\partial t} + \nabla_{\mathbf{x}}\cdot(c\rho_B\mathbf{v}_B) &= \Pi_\rho\,,\\
\frac{\partial}{\partial t}[(1-c)\rho_L v_L^j] + \nabla_{\mathbf{x}}\cdot[(1-c)\rho_L v_L^j\mathbf{v}_L] + \frac{\partial(1-c)p_L}{\partial x_j} - (1-c)\rho_L g^j &= -\,\Pi_m^j\,,\\
\frac{\partial(c\rho_B v_B^j)}{\partial t}(t,\mathbf{x}) + \nabla_{\mathbf{x}}\cdot(c\rho_B v_B^j\mathbf{v}_B) - c\rho_B g^j &= \Pi_m^j\,,\\
\frac{\partial}{\partial t}(1-c)\rho_L e_L + \nabla_x\cdot(1-c)\left((\rho_L e_L + p_L)\mathbf{v}_L + \mathbf{Q}_L\right) - (1-c)\rho_L\,\mathbf{g}\cdot\mathbf{v}_L &= -\,\Pi_e\,,\\
\frac{\partial c\rho_B e_B}{\partial t} + \nabla_{\mathbf{x}}\cdot(c\rho_B e_B\mathbf{v}_B) - c\rho_B\,\mathbf{g}\cdot\mathbf{v}_B &= \Pi_e\,.
\end{aligned} \tag{50}$$

Using (46), the balance equation for the number density can easily be rewritten in terms of the more descriptive quantity R. We obtain

$$\frac{\partial cR}{\partial t} + \nabla_{\mathbf{x}}\cdot(cR\mathbf{v}_B) = \frac{4}{3}R\Pi_c\,.$$

With the definition $\Pi_R := 4c\dot{R}$, we give the alternative system (51) of 8 partial differential equations for the determination of the variables mean bubble radius R, volume fraction of the disperse phase c, densities of the phases ρ_L, ρ_B, velocities of the phases $\mathbf{v}_L$, $\mathbf{v}_B$ and energy of the phases e_L, e_B

$$
\begin{aligned}
\frac{\partial cR}{\partial t} + \nabla_{\mathbf{x}} \cdot (cR\mathbf{v}_B) =& \Pi_R\,, \\
\frac{\partial c}{\partial t} + \nabla_{\mathbf{x}} \cdot (c\,\mathbf{v}_B) =& \Pi_c\,, \\
\frac{\partial}{\partial t}[(1-c)\rho_L] + \nabla_{\mathbf{x}} \cdot [(1-c)\rho_L \mathbf{v}_L] =& -\Pi_\rho\,, \\
\frac{\partial c\rho_B}{\partial t} + \nabla_{\mathbf{x}} \cdot (c\,\rho_B \mathbf{v}_B) =& \Pi_\rho\,, \\
\frac{\partial}{\partial t}[(1-c)\rho_L v_L^j] + \nabla_{\mathbf{x}} \cdot [(1-c)\rho_L v_L^j \mathbf{v}_L] + \frac{\partial (1-c)p_L}{\partial x_j} - (1-c)\rho_L g^j =& -\Pi_m^j\,, \\
\frac{\partial (c\rho_B v_B^j)}{\partial t}(t,\mathbf{x}) + \nabla_{\mathbf{x}} \cdot (c\,\rho_B v_B^j \mathbf{v}_B) - c\rho_B g^j =& \Pi_m^j\,, \\
\frac{\partial}{\partial t}(1-c)\rho_L e_L + \nabla_x \cdot (1-c)\left((\rho_L e_L + p_L)\mathbf{v}_L + \mathbf{Q}_L\right) - (1-c)\rho_L\,\mathbf{g}\cdot\mathbf{v}_L =& -\Pi_e\,, \\
\frac{\partial c\rho_B e_B}{\partial t} + \nabla_{\mathbf{x}} \cdot (c\rho_B e_B \mathbf{v}_B) - c\rho_B\,\mathbf{g}\cdot\mathbf{v}_B =& \Pi_e\,.
\end{aligned}
\tag{51}
$$

Finally it remains to give the equation of state for the liquid pressure. The averaging process is simple here. It relies on the corresponding microscopic equation of state (28)

$$
(1-c)p_L = (1-c)\overline{\left[p_{ref} + K(\rho/\rho_{ref} - 1)\right]} = (1-c)\left[p_{ref} + K(\rho_L/\rho_{ref} - 1)\right]
$$

since p_{ref}, K and ρ_{ref} are constants giving a linear relation between ρ and p.

The volume fraction of the carrier phase is always taken to be $1-c$ and does not need to be determined. To solve the system presented one needs a complete set of initial data. In addition to the initial data for the unknowns in (50), we need initial data for $\dot{R}$. Analogously to previous calculations these data can be found using

$$
\dot{R}(t) = \frac{\sum_\alpha R_\alpha^2(t)\dot{R}_\alpha(t)\,\chi_a(\mathbf{x} - \mathbf{q}_\alpha(t))}{c/R(t,\mathbf{x})} \tag{52}
$$

at $t=0$, which results from the averaging of the change of volume density, see also the following sections.

Next we will explicitly study four problems, in which simplified flows are involved. To illustrate clearly, how to deal with the source terms resp. evolution laws, we restrict ourselves to the isothermal subproblem for a single spherical bubble. First we investigate the mathematical properties of the resulting model in Section 5. Several evolution laws are available for the computation of $\dot{R}$, $\dot{m}$ and $\dot{T}$, see [4]. In Section 6 we summarize the results of [4] and we explain their application to the system (50). Numerical results are then presented in Section 7.

5 Mathematical properties of the radial symmetric system

Considering spherical symmetry and assuming an isothermal process we get the simplest case. This means that we have a bubble with its center in the origin which gives us some test cases for comparisons with the results of our paper [4].

As already mentioned, the gravity terms drop out, further $\Pi_m = 0$ and the energy balances become redundant. The system corresponding to (50) consists of 6 equations of the following form

$$\begin{aligned}
\frac{\partial c}{\partial t} + \frac{\partial c v_B}{\partial r} &= -\frac{2}{r} c v_B + \Pi_c && (53)\\
\frac{\partial cn}{\partial t} + \frac{\partial c n v_B}{\partial r} &= -\frac{2}{r} cR v_B && (54)\\
\frac{\partial c\rho_B}{\partial t} + \frac{\partial c\rho_B v_B}{\partial r} &= -\frac{2}{r} c\rho_B v_B + \Pi_\rho && (55)\\
\frac{\partial c\rho_B v_B}{\partial t} + \frac{\partial c\rho_B v_B^2}{\partial r} &= -\frac{2}{r} c\rho_B v_B^2 && (56)\\
\frac{\partial (1-c)\rho_L}{\partial t} + \frac{\partial (1-c)\rho_L v_L}{\partial r} &= -\frac{2}{r}(1-c)\rho_L v_L - \Pi_\rho && (57)\\
\frac{\partial (1-c)\rho_L v_L}{\partial t} + \frac{\partial (1-c)\rho_L v_L^2}{\partial r} + \frac{\partial (1-c) p_L}{\partial r} &= -\frac{2}{r}(1-c)\rho_L v_L^2 . && (58)
\end{aligned}$$

Due to the radial symmetry, one obtains additional geometric source terms on the right hand side of the equations. All sources are non-differential, this means, that the system is in divergence form in contrast to other two-phase models, see for instance Baer and Nunziato [2] or Stewart and Wendroff [19].

For a single bubble in the origin it must hold that $v_B(t,r) = 0$ for all t. Indeed, this is the unique solution of the above system with the initial data $v_B(0,r) = 0$. With $v_B(t,r) = 0$ for all t equation (54) reduces to $\frac{\partial cn}{\partial t} = 0$ and becomes redundant for given initial data $n(0,r)$. Further, the equation (56) drops out. The system (53-58) reduces to a system of only 4 equations of the much more simple form

$$\begin{aligned}
\frac{\partial c}{\partial t} &= \Pi_c && (59)\\
\frac{\partial c\rho_B}{\partial t} &= \Pi_\rho && (60)\\
\frac{\partial (1-c)\rho_L}{\partial t} + \frac{\partial (1-c)\rho_L v_L}{\partial r} &= -\frac{2}{r}(1-c)\rho_L v_L - \Pi_\rho && (61)\\
\frac{\partial (1-c)\rho_L v_L}{\partial t} + \frac{\partial (1-c)\rho_L v_L^2}{\partial r} + \frac{\partial (1-c) p_L}{\partial r} &= -\frac{2}{r}(1-c)\rho_L v_L^2 . && (62)
\end{aligned}$$

The non-differential sources on the right hand side do not influence the mathematical type of the system. Therefore it is sufficient to investigate the homogeneous system. Using $\frac{\partial p_L}{\partial \rho_L} = \frac{a_L^2}{\rho_L}$ with the sound speed a_L of the liquid for convenience we write the homogeneous system in primitive variables

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{A}(\mathbf{u}) \frac{\partial \mathbf{u}}{\partial r} = \mathbf{0},$$

where $\mathbf{u} = (c, \rho_B, \rho_L, v_L)^T$ denotes the independent unknowns. The matrix $\mathbf{A}$ is given by

$$\mathbf{A} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -\frac{\rho_L v_L}{1-c} & 0 & v_L & \rho_L \\ -\frac{p_L}{(1-c)\rho_L} & 0 & \frac{a_L^2}{\rho_L} & v_L \end{pmatrix} \tag{63}$$

with $p_L = p_{ref} + K(\rho_{ref}/\rho_L - 1)$. After some simple calculations one gets the eigenvalues of $\mathbf{A}$ as

$$\lambda_1 = v_L - a_L \quad \lambda_2 = \lambda_3 = 0 (= v_B) \quad \lambda_4 = v_L + a_L. \tag{64}$$

and 4 corresponding linearly independent eigenvectors

$$\mathbf{e}_1 = \begin{pmatrix} 0 \\ 0 \\ -\frac{\rho_L}{a_L} \\ 1 \end{pmatrix} \quad \mathbf{e}_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \quad \mathbf{e}_3 = \begin{pmatrix} \frac{a_L^2 - v_L^2}{p_L - \rho_L v_L^2}(1-c) \\ 0 \\ 1 \\ \frac{v_L}{\rho_L} \frac{\rho_L a_L^2 - p_L}{p_L - \rho_L v_L^2} \end{pmatrix} \quad \mathbf{e}_4 = \begin{pmatrix} 0 \\ 0 \\ \frac{\rho_L}{a_L} \\ 1 \end{pmatrix}. \tag{65}$$

Obviously, the system is non-strictly hyperbolic.

Considering a Riemann problem one obtains the Riemann invariants c, ρ_B of a 1-wave and the 4-wave. This means, that these quantities do not change across the 1- and 4-wave. For the double eigenvalue $\lambda = 0$ one has a contact discontinuity. Here all quantities change. The Riemann invariants are given by

$$(1-c)\rho_L v_L = \text{const} \qquad \text{and} \quad (1-c)(\rho_L v_L^2 + p_L) = \text{const}. \tag{66}$$

Remark 1. *If one further excludes phase transition, then we have $\Pi_\rho = 0$ and the bubble mass balance becomes redundant as well for given initial data $\rho_B(0, r)$. The system reduces to the equations (59), (61), and (62). In the Jacobian matrix $\mathbf{A}$ the second row and column drop out and one obtains the eigenvalues*

$$\lambda_1 = v_L - a_L \quad \lambda_2 = 0 (= v_B) \quad \lambda_3 = v_L + a_L$$

and the corresponding eigenvectors

$$\mathbf{e}_1 = \begin{pmatrix} 0 \\ -\frac{\rho_L}{a_L} \\ 1 \end{pmatrix} \quad \mathbf{e}_2 = \begin{pmatrix} \frac{a_L^2 - v_L^2}{p_L - \rho_L v_L^2}(1-c) \\ 1 \\ \frac{v_L}{\rho_L} \frac{\rho_L a_L^2 - p_L}{p_L - \rho_L v_L^2} \end{pmatrix} \quad \mathbf{e}_3 = \begin{pmatrix} 0 \\ \frac{\rho_L}{a_L} \\ 1 \end{pmatrix}.$$

The system is strictly hyperbolic with the Riemann invariant c of the 1- and 3- wave. For the eigenvalue $\lambda = 0$ one has a contact discontinuity with the same Riemann invariants as above, see (66).

6 Production terms

In order to calculate the production terms $(49)_1$, $(49)_2$, and (48), we need evolution laws for the radius $\dot{R}$ as well as the total mass $\dot{m}$ of a single bubble. In [4] several models for a single bubble system were derived. These models take into account resp. neglect the effects of mass transfer, heat conduction, and compressibility of the surrounding liquid according to various choices one can make.

To model the production terms in the paper at hand we use isothermal models for a pure water vapor bubble, see [4]. To derive such a model one assumes a single pure water vapor bubble in a sufficiently large domain, surrounded by pure liquid water. For simplicity we assume spherical symmetry and homogeneity in the vapor phase. This means that the density ρ_B, and consequently the pressure, depends only on time and is constant in space.

The mass transfer is described by a kinetic relation, based on the classical Hertz-Knudsen theory. For details we refer to Section 2 in [4]. With the further assumption of incompressible liquid water, the evolution of the bubble can be described by the following system of ordinary differential equations

$$\dot{m} = \frac{4\pi R^2 \rho_B m_0}{\sqrt{2\pi m_0 kT}} \left[\frac{1}{\rho_L} \left(\frac{\rho_B kT}{m_0} - \frac{2\sigma}{R} - \bar{p} \right) - \frac{kT}{m_0} \ln \frac{\rho_B kT}{\bar{p} m_0} - \frac{1}{2} \left(\frac{1}{\rho_L} - \frac{1}{\rho_B} \right)^2 \left(\frac{\dot{m}}{4\pi R^2} \right)^2 \right], \tag{67}$$

$$\dot{F} = \frac{F^2}{2R^3} - \frac{R}{\rho_L} \left(p_0 - \frac{\rho_B kT}{m_0} + \frac{2\sigma}{R} + \left(\frac{1}{\rho_L} - \frac{1}{\rho_B} \right) \left(\frac{\dot{m}}{4\pi R^2} \right)^2 \right), \tag{68}$$

$$\dot{R} = \frac{F}{R^2} + \frac{\dot{m}}{4\pi R^2 \rho_L}. \tag{69}$$

This is a special case of Case 2 in [4]. There a mixture of water vapor and an inert gas is assumed. The dot $\dot{}$ denotes the time derivative.

Using (67) one can calculate $\dot{m}$. The equation (67) is quadratic. The positive root gives the solution. To solve this system of ordinary differential equations one needs values for R, ρ_B and ρ_L. The values ρ_B and ρ_L are given by the values of the system (59-62) of partial differential equations. As mentioned before the averaged volume V is given by $V = 1/n$. Therefore, the averaged radius R can be calculated using $R = \sqrt[3]{\frac{3}{4\pi n}}$. In our case we have $\frac{\partial cn}{\partial t} = 0$. This means that

$$R = R_0 \sqrt[3]{\frac{c}{c_0}} \qquad \text{with} \qquad R_0 = \sqrt[3]{\frac{3}{4\pi n_0}}.$$

Further one needs the mass of a single water molecule m_0, the Boltzmann constant k, the outer pressure p_0, the temperature T, and the reference values for the surficial tension σ of water as well as for the saturation pressure $\bar{p}$ corresponding to T.

For a complete set of initial data one needs initial values for $\dot{R}$, see (52). Alternatively one can assume the system initially to be at rest and set $F(0) = 0$. This implies initial data for $\dot{R}$.

For F we have $F = v_L^I \cdot R^2$, see [4]. Using (68) and for instance a Runge-Kutta method one gets values for F in a new time step. Using (67) together with equation (69) gives values for $\dot{R}$.

In [4] it was shown, that for *large* pressure differences the compressibility of the liquid plays an important role. Taking into account compressibility of the liquid in a weak sense, one starts with the linearized Euler equations and obtains a wave equation. Its solution we denote by Φ. Assuming that the domain is large enough that the bubble is not affected by reflections at the outer boundary, one derives instead of (68) and (69) the following equations

$$\Phi'(R-a_L t) = \frac{R}{\rho_L a_L}\left(\frac{\rho_B kT}{m_0} - \frac{2\sigma}{R} - \left(\frac{1}{\rho_L} - \frac{1}{\rho_B}\right)\left(\frac{\dot{m}}{4\pi R^2}\right)^2 - p_0\right) \tag{70}$$

$$\dot{R} = -\frac{\Phi(R-a_L t)}{R^2} + \frac{\Phi'(R-a_L t)}{R} + \frac{\dot{m}}{4\pi R^2 \rho_L}, \tag{71}$$

where a_L denotes the speed of sound in the liquid. As before $\dot{}$ denotes the time derivative, whereas $'$ denotes the derivative for the argument.

Instead of (67) one gets

$$\begin{aligned}\dot{m} = \frac{4\pi R^2 \rho_B m_0}{\sqrt{2\pi m_0 kT}}\Bigg[&\frac{K}{\rho_L}\ln\left(1 + \frac{\frac{\rho_B kT}{m_0} - \frac{2\sigma}{R} - \left(\frac{1}{\rho_L} - \frac{1}{\rho_B}\right)\left(\frac{\dot{m}}{4\pi R^2}\right)^2}{K}\right) \\ &-\frac{kT}{m_0}\ln\frac{\rho_B kT}{m_0 \bar{p}} + \left(\frac{1}{\rho_L^2} - \frac{1}{\rho_B^2}\right)\left(\frac{\dot{m}}{4\pi R^2}\right)^2\Bigg]\end{aligned} \tag{72}$$

with the liquid bulk modulus K. Because of the logarithm term this equation is transcendent. The calculation of $\dot{m}$ by an iterative method is expensive. Further one has to discuss the non-uniqueness, what is unnecessarily complicated here. By linearization of the logarithm term one obtains equation (67), which is a sufficiently good approximation.

Therefore for a compressible model we use the equations (67), (70) and (71). In that case we need initial data for Φ.

Now we have two models taking into account phase transition to calculate the production terms in (59-62). If we exclude mass transfer we have $\dot{m} = 0$. The equations (68) and (69) resp. (70) and (71) then simplify.

7 Numerical results

For the current section we choose specific initial data. For these data we give numerical results for the two systems (67), (68), (69) resp. (67), (70), (71) of ordinary differential equations, in each case with and without phase transition. This gives us four test cases.

With the same initial data we solve the system (59-62) of partial differential equations for the radial symmetric case numerically and compare these results with the previous for all the four test cases.

7.1 Initial data

Let us assume a pure water vapor bubble in the origin surrounded by pure liquid water. This means, for the midpoint of the bubble we have $r = 0$ where r denotes the space coordinate. The outer boundary is chosen to be at $r = R_A = 0.3m$. This guaranties that the bubble is not affected by reflections at the outer boundary during the computation time. The temperature T is assumed to be $T = 293.15K$ and the outer pressure p_0 is the atmospheric pressure, $p_0 = 101300Pa$. Corresponding to T we give the reference values for the surficial tension $\sigma = 0.0725N/m$ and the saturation pressure $\bar{p} = 2330Pa$, see [8] or [25]. The mass of one water molecule is given by $m_0 = 2.9915 \cdot 10^{-26}kg$ and the Boltzmann constant by $k = 1.380658 \cdot 10^{-23}J/K$. Beside this we need the liquid bulk modulus K, which we chose to be $K = 2.08 \cdot 10^9 Pa$.

We choose the initial radius $R(0) = R_0 = 6 \cdot 10^{-4}m$ and assume that the bubble contains 10^{16} water molecules. Therefore the initial bubble mass is given by $m(0) = 2.9915 \cdot 10^{-10}kg$. Whereas, the initial bubble density is given by $\rho_B(0) = 0.3306kg/m^3$.

Further, in the beginning the system is assumed to be at rest. This means that the liquid velocity $v_L(0)$ equals to zero everywhere. Especially at the interface, we have $v_L^I(0) = 0$. For the incompressible case $v_L^I = F/R^2$ holds, see [4]. We have $F(0) = 0$. According to the compressible case we have $\Phi(R(0)) = 0$.

7.1.1 Initial data for the averaged system (59-62)

The derivation of the corresponding initial data for the system (59-62) of partial differential equations for constant or piecewise constant data is quite simple. For that we need the formulas (3) and (4) as well as the radius R_a of the averaging ball. We choose $R_a = 5 \cdot R_0 = 3 \cdot 10^{-3}m$. For the concentration we get $c = 0.0008$ for $0 \leq r \leq 3 \cdot 10^{-3}m$ and $c = 0$ otherwise. For numerical aspects we choose $c = 10^{-8}$ instead of $c = 0$.

The computation of the initial data for the densities ρ_B, ρ_L, and the velocity v_L is trivial. We summarize the initial data in the neighborhood of the bubble in Figure 1. Besides the plots for the four unknowns c, ρ_B, ρ_L, v_L, we give plots for the averaged radius R and the liquid pressure p_L.

7.2 Numerical results for the ODE-systems

For the initial data given in the previous subsection we now want to calculate numerical results for the four test cases. We use a Runge-Kutta method method and obtain for the two cases without phase transition the results presented in Figure 2. In the case of an incompressible liquid one obtains an undamped oscillation for the evolution of the bubble radius, for a compressible liquid the oscillation is damped.

Taking into account mass transfer, it is clear from the physics of this situation that the bubble vanishes, see [4]. The numerical results for the test cases with phase transition are given in the following Figure 3.

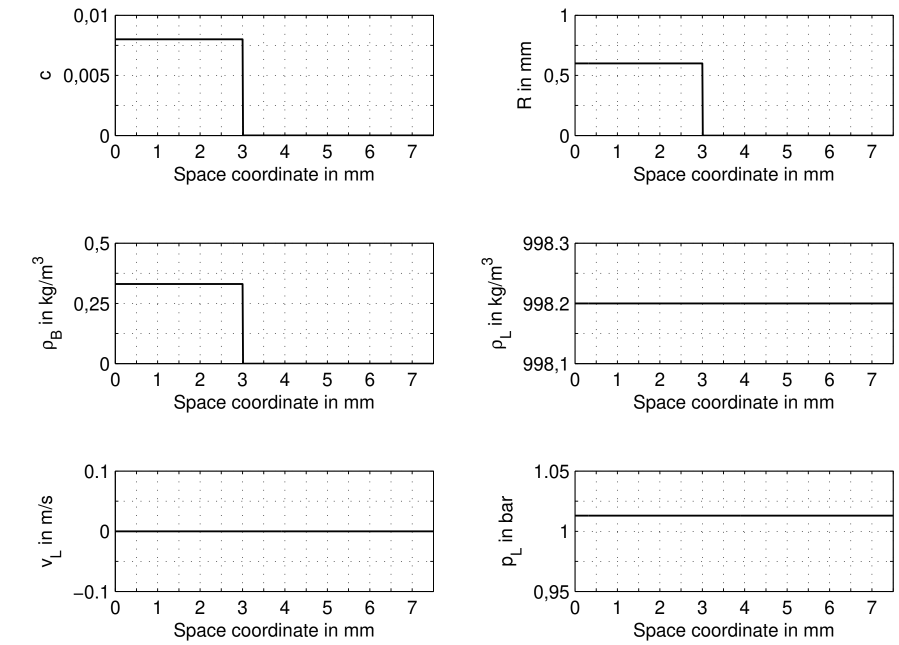

Figure 1: Initial data for (59-62) in the neighborhood of the bubble

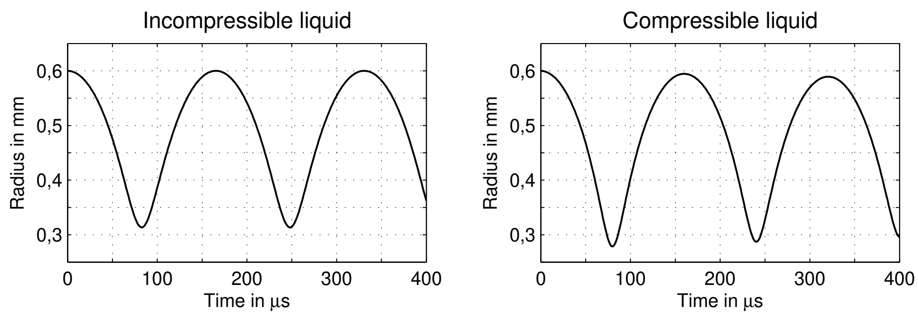

Figure 2: Bubble radius vs. time without phase transition, ODE-system

7.3 Numerical results for the averaged system (59-62)

To solve the system (59-62) numerically we use Godunov operator splitting, see Toro [20], and further a Roe type Riemann solver for the homogeneous part of the system. For the latter finite volume method we follow the procedure in [1] resp. [7].

We denote the conserved variables $c, c\rho_B, (1-c)\rho_L, (1-c)\rho_L v_L$ by $\mathbf{v}$. Then the system (59-62) can be written in the form

$$\mathbf{v}_t + \mathbf{F}(\mathbf{v})_r = \mathbf{S}(\mathbf{v}) \qquad \text{with} \qquad \mathbf{v}(t^n, r) = \mathbf{v}^n.$$

The vector $\mathbf{S}(\mathbf{v})$ denotes the sources. By the splitting procedure one first solves the homogeneous part

$$\mathbf{v}_t + \mathbf{F}(\mathbf{v})_r = 0 \qquad \text{with} \qquad \mathbf{v}(t^n, r) = \mathbf{v}^n, \tag{73}$$

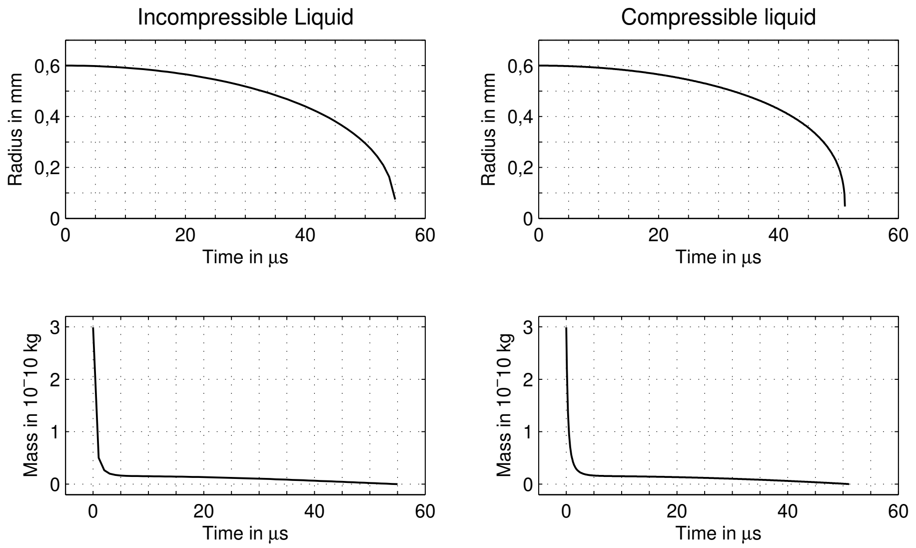

Figure 3: Bubble radius and bubble mass vs. time with phase transition, ODE-system

to obtain $\overline{\mathbf{v}}^{n+1}$. In a second step one determines

$$\frac{d}{dt}\mathbf{v} = \mathbf{S}(\mathbf{v})$$

with initial data $\overline{\mathbf{v}}^{n+1}$ to obtain the data for the new time step $\mathbf{v}^{n+1}$.

To solve the homogeneous system (73) numerically, we again as in Section 5 rewrite the system in primitive variables $\mathbf{u}$

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{A}(\mathbf{u})\frac{\partial u}{\partial r} = \mathbf{0}, \tag{74}$$

where $\mathbf{A}(\mathbf{u})$ is given in (63) and $\mathbf{u} = (c, \rho_B, \rho_L, v_L)^T$. At each cell boundary $r_{j+1/2}$ we consider the Riemann problem for (74) with initial data

$$\mathbf{u}(0,r) = \begin{cases} \mathbf{u}_j & r \leq r_{j+1/2} \\ \mathbf{u}_{j+1} & r > r_{j+1/2}\,. \end{cases}$$

We calculate the Jacobian $\mathbf{A}(\overline{\mathbf{u}})$ in the average state $\overline{\mathbf{u}}_{j+1/2} = (\mathbf{u}_j + \mathbf{u}_{j+1})/2$. By eigenvector decomposition of $\mathbf{u}_{j+1} - \mathbf{u}_j$

$$\Delta\mathbf{u} = \mathbf{u}_{j+1} - \mathbf{u}_j = \sum_{n=1}^{4} x_n \mathbf{e}_n$$

we determine the coefficients x_n to find the intermediate state

$$\mathbf{u}^*_{j+1/2} = \mathbf{u}_j + \sum_{\lambda_n < 0} x_n \mathbf{e}_n$$

in the solution of the above Riemann problem, where the eigenvalues λ_n resp. eigenvectors $\mathbf{e}_n$

of $\mathbf{A}$ are given in (64) resp. (65). We get

$$\begin{aligned}
x_1 &= \frac{-\Delta\rho_L + \frac{\rho_L}{a_L}\Delta v_L + \frac{\Delta c}{1-c}\frac{1}{a_L}\frac{p_L - \rho_L a_L v_L}{a_L - v_L}}{2\rho_L/a_L} \\
x_2 &= \Delta\rho_B \\
x_3 &= \frac{\Delta c}{1-c}\frac{p_L - \rho_L v_L^2}{a_L^2 - v_L^2} \\
x_4 &= \frac{\Delta\rho_L + \frac{\rho_L}{a_L}\Delta v_L - \frac{\Delta c}{1-c}\frac{1}{a_L}\frac{p_L - \rho_L a_L v_L}{a_L - v_L}}{2\rho_L/a_L} .
\end{aligned}$$

Using the values $\mathbf{u}^*$ in a Finite Volume method we calculate approximations $\overline{\mathbf{V}}^{n+1}$ for $\overline{\mathbf{v}}^{n+1}$

$$\overline{\mathbf{V}}^{n+1} = \overline{\mathbf{v}}^n - \frac{\Delta t}{\Delta r}\left[\mathbf{v}(\mathbf{u}^+)^n_{j+1/2} - \mathbf{v}(\mathbf{u}^*)^n_{j-1/2}\right] .$$

Remark 2. *If we exclude phase transition the above calculations simplify according to Section 5.*

Finally, for the source term integration we again use the explicit Euler method. For our calculations we chose a CFL number of 0.9 and a spatial step size of $\Delta r = 1.2 \cdot 10^-5m$ and compute the following results. Note, that we do not plot the whole computational domain but only the bubble and its neighborhood. Obviously the solutions for the radius evolution of the ODE systems

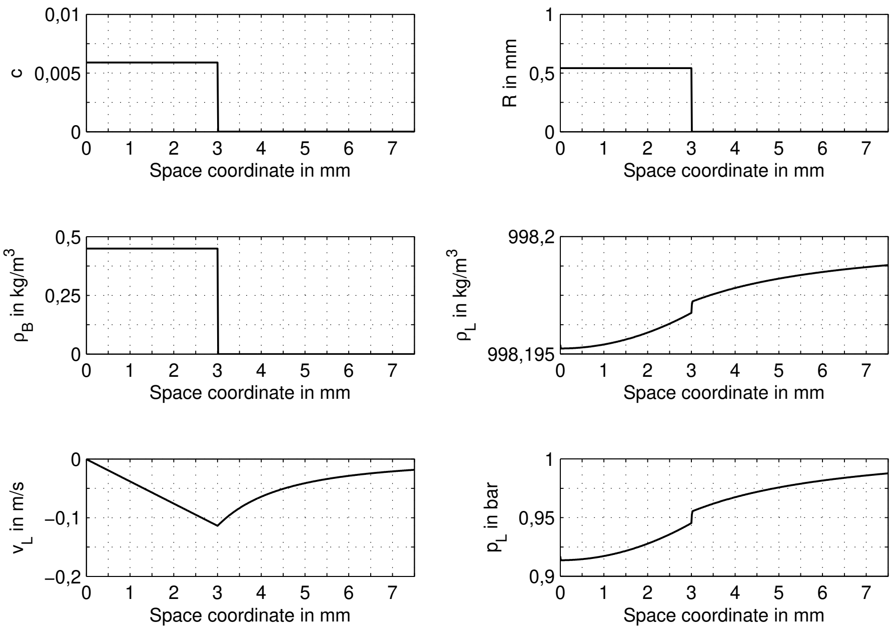

Figure 4: Numerical solution for $t = 40\mu s$, incompressible liquid without phase transition

are in very good agreement with the solutions of the averaged system with the corresponding sources.

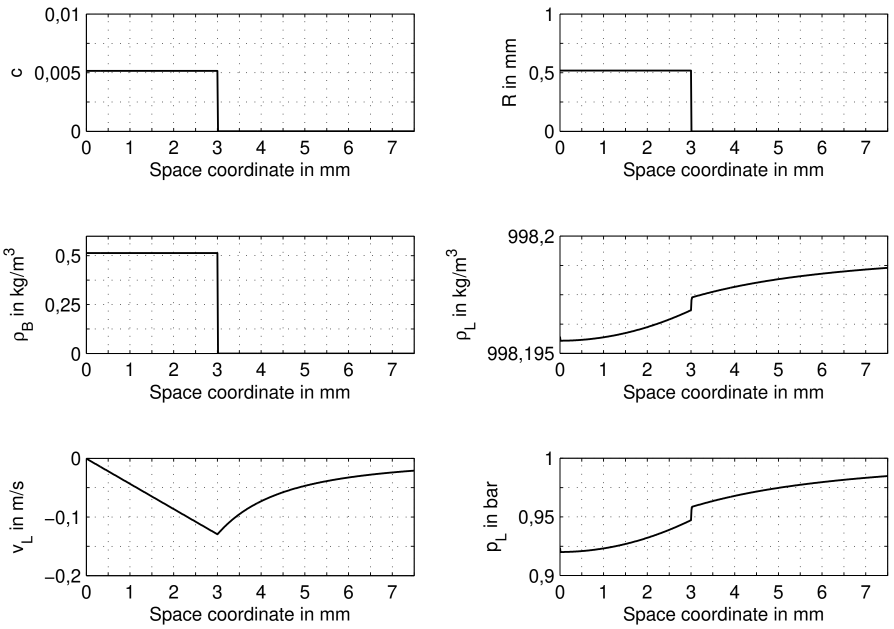

Figure 5: Numerical solution for $t = 40\mu s$, compressible liquid without phase transition

A Appendix: Newton's second law with non-constant mass

Most textbook examples in classical mechanics deal only with the dynamics of bodies with constant mass. The following argument is taken mostly from Müller [15, Subsection 1.4.6]. Consider a closed system of a rocket R emitting burnt gases B. The masses m_R of the rocket and m_B of the burnt gas are changing in time. The burning rate is $-\dot{m}_R$. Let v be the constant speed relative to the rocket of the gas emitted in the direction of an axis chosen parallel to the movement of the rocket. Let v_R be the speed of the rocket along this axis. The speed of the burnt gas in the resting frame satisfies $v_B = v_R - v$. We have mass conservation $\dot{m}_R(t) + \dot{m}_B(t) = 0$. The total momentum of the burnt gas is given as

$$m_B v_B = -\int_{t_0}^{t} \dot{m}_R(\tau)(v_R(\tau) - v)\, d\tau.$$

Momentum conservation states that

$$0 = \frac{d}{dt}(m_R v_R + m_B v_B) = \dot{m}_R v_R + m_R \dot{v}_R - \frac{d}{dt}\int_{t_0}^{t} \dot{m}_R(\tau)(v_R(\tau) - v)\, d\tau$$

The fundamental theorem of calculus gives

$$0 = \dot{m}_R v_R + m_R \dot{v}_R - \dot{m}_R(t)(v_R(t) - v) = m_R \dot{v}_R + \dot{m}_R v.$$

This implies

$$m_R(t)\dot{v}_R(t) = -\dot{m}_R(t) v$$

i.e. the thrust of the rocket is $\Theta = -\dot{m}_R v$. The above equation leads to

$$\frac{d}{dt}(m_R v_R) = \dot{m}_R v_R + m_R \dot{v}_R = \dot{m}_R(v_R - v) = \dot{m}_R v_B.$$

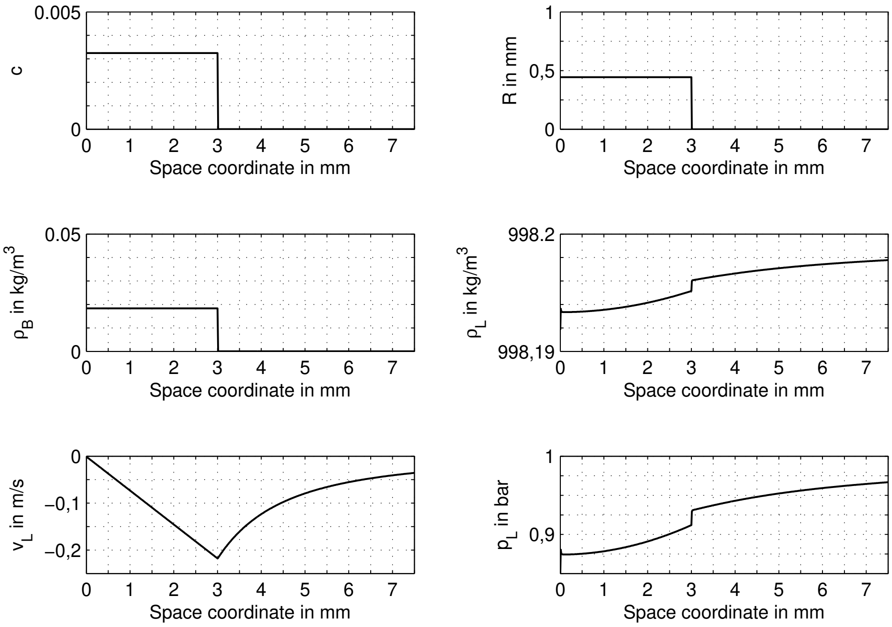

Figure 6: Numerical solution for $t = 40\mu s$, incompressible liquid with phase transition

Identifying the particles with the rocket and the carrier phase with the burnt gas the term on the right hand side motivates the last term in (32).

B Appendix: Distributional derivatives

For the definition of distributional derivatives see e.g. Hörmander [9, Chapter 2], Warnecke [21, Appendix C]. Here we first consider the case of superposition of functions $f \in L^1_{loc}(\mathbb{R}^3)$ with $f(\mathbf{x} - \mathbf{q}(t))$ for a smooth vector field $\mathbf{q} \in \mathbb{R}^3$ needed in proofs of Section 2. We consider this

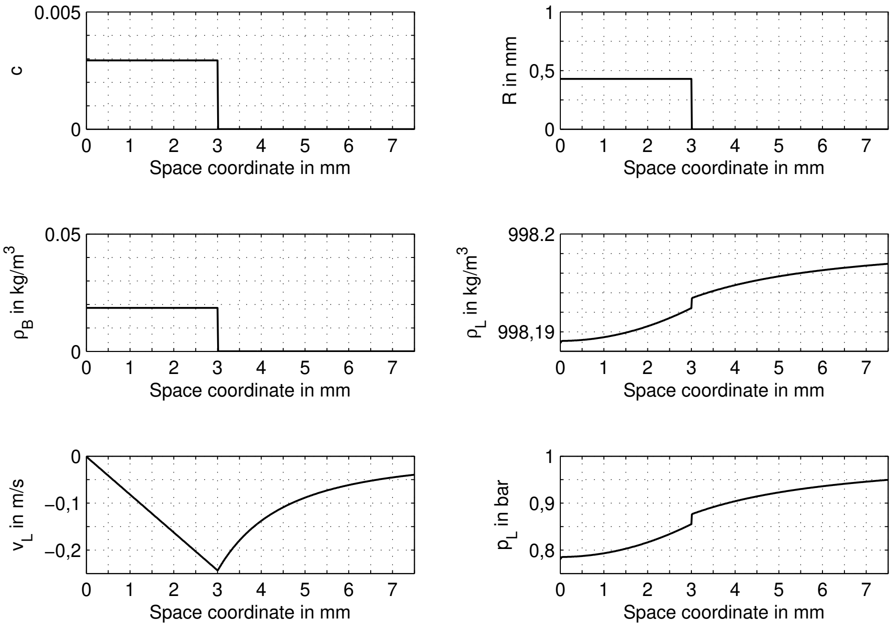

Figure 7: Numerical solution for $t = 40\mu s$, compressible liquid with phase transition

as a distribution in $\mathbb{R}^4$. Take $\phi \in C_0^\infty(\mathbb{R}^4)$ then

$$
\begin{aligned}
\langle \frac{d}{dt} f(\cdot - \mathbf{q}(t))\,,\, \phi \,\rangle &= -\,\langle\, f(\cdot - \mathbf{q}(t))\,,\, \frac{\partial}{\partial t}\phi \,\rangle \\
&= -\int_{\mathbb{R}^4} f(\mathbf{x} - \mathbf{q}(t)) \frac{\partial}{\partial t}\phi(t,\mathbf{x})\, dt\, d\mathbf{x} \\
&= -\int_{\mathbb{R}^4} f(y) \frac{\partial}{\partial t}\phi(t, y + \mathbf{q}(t))\, dt\, dy \\
&= -\int_{\mathbb{R}^4} f(y) \left[\frac{d}{dt}\phi(t, y + \mathbf{q}(t)) - \nabla_y \phi(t, y + \mathbf{q}(t)) \cdot \dot{\mathbf{q}} \right] dt\, dy \\
&= \int_{\mathbb{R}^4} f(y) \nabla_y \phi(t, y + \mathbf{q}(t)) \cdot \dot{\mathbf{q}}\, dt\, dy \\
&= \int_{\mathbb{R}^4} f(\mathbf{x} - \mathbf{q}(t)) \dot{\mathbf{q}} \cdot \nabla_{\mathbf{x}} \phi(t,\mathbf{x})\, dt\, d\mathbf{x} \\
&= \langle\, f(\cdot - \mathbf{q}(t)) \dot{\mathbf{q}}\,,\, \nabla\phi \,\rangle \\
&= -\,\langle\, \nabla_{\mathbf{x}} f(\cdot - \mathbf{q}(t)) \cdot \dot{\mathbf{q}}\,,\, \phi \,\rangle.
\end{aligned}
$$

The derivative $\nabla_{\mathbf{x}}\, \chi_a(\mathbf{x} - \mathbf{x}')$ has to be taken in the sense of distributions on $\mathbb{R}^3$ and is a singular signed vector measure $\boldsymbol{\mu}_{\partial B_a(\mathbf{x})}$ on the boundary $\partial B_a(\mathbf{x})$ with mass $-\boldsymbol{\eta}$ given by the

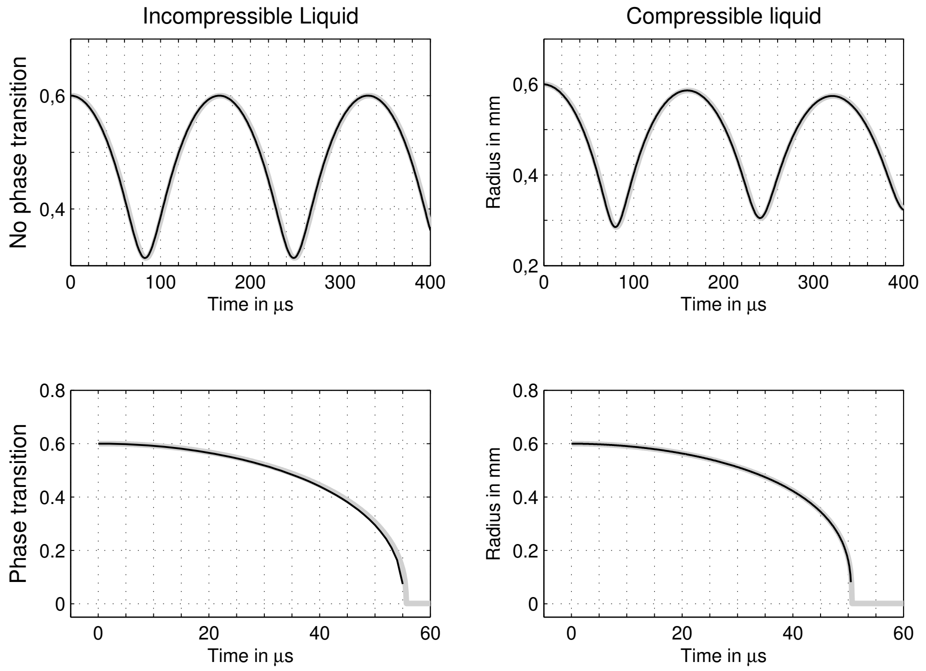

Figure 8: Radius vs. time, compressible and incompressible liquid, with and without phase transition, grey: solution of the PDE-system, black: solution of the ODE-system

outer normal. Take $\phi \in C_0^\infty(\mathbb{R}^3)$ then

$$\begin{aligned}
\langle \frac{\partial}{\partial x^j}\, \chi_a(\cdot - \mathbf{x}'), \phi \rangle &= -\langle \chi_a(\cdot - \mathbf{x}'), \frac{\partial}{\partial x^j}\phi \rangle = -\int_{\mathbb{R}^3} \chi_a(\mathbf{x}-\mathbf{x}') \frac{\partial}{\partial x^j}\phi(\mathbf{x})\, d\mathbf{x} \\
&= -\int_{B_a(\mathbf{x}')} \frac{\partial}{\partial x^j}\phi(\mathbf{x})\, d\mathbf{x} = -\int_{\partial B_a(\mathbf{x}')} \eta^j \phi(\mathbf{x})\, d\mathbf{x} \\
&= \int_{\mathbb{R}^3} \phi(\mathbf{x})\, d\mu^j_{\partial B_a(\mathbf{x}')} = \langle \mu^j_{\partial B_a(\mathbf{x}')}, \phi \rangle.
\end{aligned}$$

Now we derive the *shift of differentiation formula* that we needed in the proof of the general transport equation in Lemma 3. We consider arbitrary test functions $\phi^{\mathbf{x}}, \psi^{\mathbf{x}'} \in C_0^\infty(\mathbb{R}^3)$, use a change of variables and integration by parts to get

$$\begin{aligned}
\langle \frac{\partial}{\partial(\mathbf{x}')^j}\,\chi_a\,,\,\phi^{\mathbf{x}}\psi^{\mathbf{x}'}\,\rangle &= -\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\chi_a(\mathbf{x}-\mathbf{x}')\frac{\partial}{\partial(\mathbf{x}')^j}\psi^{\mathbf{x}'}(\mathbf{x}')\,d\mathbf{x}'\,\phi^{\mathbf{x}}(\mathbf{x})\,d\mathbf{x} \\
&= \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\chi_a(y)\frac{\partial}{\partial x^j}\psi^{\mathbf{x}'}(\mathbf{x}-\mathbf{y})\,d\mathbf{y}\,\phi^{\mathbf{x}}(\mathbf{x})\,d\mathbf{x} \\
&= \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\frac{\partial}{\partial x^j}\psi^{\mathbf{x}'}(\mathbf{x}-\mathbf{y})\phi^{\mathbf{x}}(\mathbf{x})\,d\mathbf{x}\;\chi_a(\mathbf{y})\,d\mathbf{y} \\
&= -\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\psi^{\mathbf{x}'}(\mathbf{x}-\mathbf{y})\frac{\partial}{\partial x^j}\phi^{\mathbf{x}}(\mathbf{x})\,d\mathbf{x}\;\chi_a(\mathbf{y})\,d\mathbf{y} \\
&= -\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\chi_a(\mathbf{y})\psi^{\mathbf{x}'}(\mathbf{x}-\mathbf{y})\,d\mathbf{y}\;\frac{\partial}{\partial x^j}\phi^{\mathbf{x}}(\mathbf{x})\,d\mathbf{x} \\
&= \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\chi_a(\mathbf{x}-\mathbf{x}')\psi^{\mathbf{x}'}(\mathbf{x}')\,d\mathbf{x}'\;\frac{\partial}{\partial x^j}\phi^{\mathbf{x}}(\mathbf{x})\,d\mathbf{x} \\
&= -\langle \frac{\partial}{\partial x^j}\,\chi_a\,,\,\phi^{\mathbf{x}}\psi^{\mathbf{x}'}\,\rangle.
\end{aligned}$$

C Appendix: Exterior potential flow

We take a flow domain around one ball $B_R(\mathbf{q})$ of radius R centered at the the moving point $\mathbf{q}$ with velocity $\dot{\mathbf{q}}$ at time t. Note that in this appendix R is not identical to the macroscopic field for the radius equation and here we have $\dot{R} = \frac{dR}{dt}$. We want to use this notation to conform with presentations of the exterior potential problem such as in Landau and Lifshitz [12] or Michlin [13]. We introduce the coordinates $\mathbf{x}$ to be at rest and $\mathbf{r} = \mathbf{x} - \mathbf{q}$ the moving coordinate for which we will formulate a potential. We consider a flow potential Φ satisfying the linear potential equation $\Delta\Phi = 0$ and $\mathbf{v}_\infty \cdot \mathbf{r}$ at infinity. Since $\Phi(\mathbf{r}) = |\mathbf{r}|^{-1} = r^{-1}$ is a solution to this equation outside any ball around the origin, so is any derivative. Due to Maxwell is the ansatz using derivatives of r^{-1}, see Lamb [11, Section 82], using the summation convention where indices appearing twice in a term are summed over 1,2,3,

$$\Phi(t,\mathbf{r}) = v_\infty^i r^i + A\frac{1}{r} + B^i\frac{\partial}{\partial x^i}\frac{1}{r} + C^{ij}\frac{\partial}{\partial x^i\partial x^j}\frac{1}{r} + \dots\,.$$

We will truncate the series after the B^i

$$\Phi = v_\infty^i r^i + A\frac{1}{r} + B^i\frac{\partial}{\partial x^i}\frac{1}{r}.$$

We will see that then we have enough terms to pose appropriate boundary conditions on the ball. We use

$$\frac{\partial r}{\partial x^i} = \frac{x^i - q^i}{r} = \frac{r^i}{r} \quad \text{and} \quad \text{thereby} \quad \frac{\partial r^{-1}}{\partial x^i} = -\frac{x^i - q^i}{r^3} = -\frac{r^i}{r^3}$$

to obtain

$$\Phi = v_\infty^i r^i + A\frac{1}{r} - B^i\frac{r^i}{r^3}.$$

We denote by $\mathbf{R}$ with $R = |\mathbf{R}|$ the coordinates on the surface of the ball. Then the velocity components for $j = 1,2,3$ there are given as

$$v^j\bigg|_{\mathbf{R}} = \frac{\partial \Phi}{\partial x^j}\bigg|_{\mathbf{R}} = v_\infty^j - A\frac{R^j}{R^3} + B^i\left(\frac{3R^iR^j}{R^5} - \frac{\delta_{ij}}{R^3}\right). \tag{75}$$

Using the assumption that all quantities are constant on the surface (38) gives

$$\dot{m} = -\rho_L \oint_{\partial B_R(0)} \left[\mathbf{v}(t,\mathbf{x}') - \mathbf{w}(t)\right] \cdot \boldsymbol{\eta}\, dS = -4\pi R^2 \rho_L \left[\mathbf{v} - \mathbf{w}(t)\right] \cdot \boldsymbol{\eta}.$$

Note that $\mathbf{w} = \dot{\mathbf{R}} + \dot{\mathbf{q}}$, $\boldsymbol{\eta} = \mathbf{R}/R$, and then $\dot{R} = \boldsymbol{\eta} \cdot \dot{\mathbf{R}}$ giving

$$\mathbf{v} \cdot \boldsymbol{\eta} = -\frac{\dot{m}}{4\pi\rho_L R^2} + \dot{R} + \frac{\dot{\mathbf{q}} \cdot \mathbf{R}}{R}. \tag{76}$$

Multipying $\eta^j = R^j/R$ to (75) and comparing the result with (76) we have

$$\begin{aligned} v^j\eta^j\bigg|_{\mathbf{R}} = \frac{\partial \Phi}{\partial x^j}\eta^j\bigg|_{\mathbf{R}} &= \frac{v_\infty^j R^j}{R} - \frac{A}{R^2} + B^jR^j\frac{2}{R^4} \\ &= \dot{R} - \frac{\dot{m}}{4\pi\rho_L R^2} + \dot{q}^j\frac{R^j}{R}. \end{aligned}$$

There is a unique solution to the exterior Neumann problem for the potential equation that decays to $\mathbf{v}_\infty \cdot \mathbf{r}$ like r^{-1}, see e.g. Michlin [13, Satz 13.2.2]. It can be expanded uniquely by spherical harmonics, see e.g. Michlin [13, Section 15.4]. This implies that the coefficients in our case are

$$A = \frac{\dot{m}}{4\pi\rho_L} - \dot{R}R^2, \qquad B^j = \frac{1}{2}R^3(\dot{q}^j - v_\infty^j)$$

leading to

$$\Phi(t,\mathbf{x}) = v_\infty^j r^j + \frac{\dot{m}}{4\pi\rho_L r} - \frac{\dot{R}R^2}{r} - \frac{R^3 r^j(\dot{q}^j - v_\infty^j)}{2r^3}. \tag{77}$$

We take the Bernoulli equation, see Lamb [11]

$$f(t) = \frac{\partial \Phi}{\partial t} + \frac{1}{2}\frac{\partial \Phi}{\partial x^j}\frac{\partial \Phi}{\partial x^j} + \frac{p}{\rho_L} + gx^3.$$

The aim is to determine the pressure. Using (81) we obtain

$$\begin{aligned} \frac{1}{\rho_L}\oint_{\partial B_R(0)} p\eta^i\, dS &= -\oint_{\partial B_R(0)} \left(-f(t) + \frac{1}{2}\frac{\partial \Phi}{\partial x^j}\frac{\partial \Phi}{\partial x^j} + \frac{\partial \Phi}{\partial t} + gx^3\right)\eta^i\, dS \\ &= -\oint_{\partial B_R(0)} \left(\frac{1}{2}\frac{\partial \Phi}{\partial x^j}\frac{\partial \Phi}{\partial x^j} + \frac{\partial \Phi}{\partial t} + gx^3\right)\eta^i\, dS. \end{aligned} \tag{78}$$

Now we compute the derivative terms of the potential needed in the Bernoulli equation

$$\begin{aligned}\left.\frac{\partial\Phi}{\partial x^j}\frac{\partial\Phi}{\partial x^j}\right|_R &= v_\infty^j v_\infty^j + 2v_\infty^j B^i\left(\frac{3R^iR^j}{R^5}-\frac{\delta_{ij}}{R^3}\right) - 2v_\infty^j A\frac{R^j}{R^3}\\ &\quad + A^2\frac{1}{R^4} + B^iB^k\left(\frac{3R^iR^j}{R^5}-\frac{\delta_{ij}}{R^3}\right)\left(\frac{3R^kR^j}{R^5}-\frac{\delta_{kj}}{R^3}\right) - 4AB^i\frac{R^i}{R^6}.\end{aligned}$$

We turn to the time derivative and note that

$$\frac{\partial r^j}{\partial t} = \frac{\partial}{\partial t}(x^j - q^j) = -\dot q^j.$$

This gives

$$\frac{\partial r}{\partial t} = -\frac{r^j}{r}\dot q^j$$

and we obtain

$$\begin{aligned}\left.\frac{\partial\Phi}{\partial t}\right|_R &= \left.\frac{\partial}{\partial t}\left(v_\infty^j r^j + A\frac{1}{r} - B^j\frac{r^j}{r^3}\right)\right|_R\\ &= -v_\infty^j\dot q^j + \dot A\frac{1}{R} - A\frac{1}{R^2}\left.\frac{\partial r}{\partial t}\right|_R - \dot B^j\frac{R^j}{R^3} - B^j\frac{1}{R^3}\left.\frac{\partial r^j}{\partial t}\right|_R + 3B^jR^j\frac{1}{R^4}\left.\frac{\partial r}{\partial t}\right|_R\\ &= -v_\infty^j\dot q^j + \dot A\frac{1}{R} + A\frac{R^j}{R^3}\dot q^j - \dot B^j\frac{R^j}{R^3} + B^j\frac{1}{R^3}\dot q^j - 3B^jR^jR^i\dot q^i\frac{1}{R^5}.\end{aligned}$$

The derivatives obtained are now inserted into the formula (78) for the pressure. We make use of the fact that formulae (81-83) imply that we only have to retain terms where the integrand contains a constant times the product of two normal components η^i or depends on a space variable, as in the gravitational term,

$$\begin{aligned}\frac{1}{\rho_L}\oint_{\partial B_R(0)} p\eta^i\,dS &= \oint_{\partial B_R(0)}\left(v_\infty^j A\frac{R^j}{R^3} + 2AB^j\frac{R^j}{R^6} - A\frac{R^j}{R^3}\dot q^j + \dot B^j\frac{R^j}{R^3} - g\delta_{i3}\right)\eta^i\,da\\ &= \frac{4}{3}\pi v_\infty^i A + \frac{8}{3}\pi AB^i\frac{1}{R^3} - \frac{4}{3}\pi A\dot q^i + \frac{4}{3}\pi\dot B^i - g\delta_{i3}\frac{4}{3}\pi R^3\\ &= \frac{4}{3}\pi v_\infty^i A + \frac{4}{3}\pi A(\dot q^i - v_\infty^i) - \frac{4}{3}\pi A\dot q^i + \frac{4}{3}\pi\dot B^i - g\delta_{i3}\frac{4}{3}\pi R^3\\ &= \frac{4}{3}\pi\dot B^i - g\delta_{i3}\frac{4}{3}\pi R^3\end{aligned}$$

giving

$$\begin{aligned}\oint_{\partial B_R(0)} p\eta^i\,dS &= \rho_L\left(\frac{4}{3}\pi\dot B^i - g\delta_{i3}\frac{4}{3}\pi R^3\right)\\ &= \rho_L\left(\frac{2}{3}\pi\left(R^3\dot q^i\right)^{\cdot} - 2\pi R^2\dot R v_\infty^i - g\delta_{i3}\frac{4}{3}\pi R^3\right).\end{aligned}$$

With $v_\infty^i = 0$ we obtain

$$\oint_{\partial B_R(0)} p\eta^i\,dS = \rho_L\left(\frac{2}{3}\pi\left(R^3\dot q^i\right)^{\cdot} - g\delta_{i3}\frac{4}{3}\pi R^3\right). \tag{79}$$

We compute the $\mathbf{v}$ term in (32). Note that A and the B^j are constant and contain no normal components $\eta^i = R^i/R$. Therefore we can use (81) and (82) to obtain

$$\begin{aligned}
\oint_{\partial B_R(0)} v^j\, dS &= \oint_{\partial B_R(0)} \frac{\partial \Phi}{\partial x^j}\, dS \\
&= \oint_{\partial B_R(0)} \left(v_\infty^j - A\frac{R^j}{R^3} + B^i \left(\frac{3R^iR^j}{R^5} - \frac{\delta_{ij}}{R^3} \right) \right) dS \\
&= 4\pi R^2 v_\infty^j + \oint_{\partial B_R(0)} B^i \left(\frac{3R^iR^j}{R^5} - \frac{\delta_{ij}}{R^3} \right) dS \\
&= 4\pi R^2 v_\infty^j + \frac{B^i}{R^3} \oint_{\partial B_R(0)} \left(3\frac{R^iR^j}{R^2} - \delta_{ij} \right) dS \\
&= 4\pi R^2 v_\infty^j + \frac{B^i}{R^3} \left(3\frac{4}{3}\pi R^2 - 4\pi R^2 \right) \delta_{ij} = 4\pi R^2 v_\infty^j = 0\,.
\end{aligned} \tag{80}$$

D Appendix: Surface integrals

In Appendix C we had to evaluate a number surface integrals for integrands consisting of one, two or three components of the exterior normal vector on $\partial B_R(\mathbf{q})$. For an arbitrary domain $\boldsymbol{\Omega}$ allowing the use of the Gauss theorem we have

$$\oint_{\partial\Omega} \eta^i\, dS = \int_\Omega \partial_{x^i} 1\, d\mathbf{x} = 0. \tag{81}$$

We extend the vector field $\boldsymbol{\eta} = \mathbf{R}/R$ by $(\mathbf{x}-\mathbf{q})/R$ to the interior of $B_R(\mathbf{q})$

$$\oint_{\partial B_R(\mathbf{q})} \eta^i \eta^j\, dS = \int_{B_R(\mathbf{q})} \partial_{x^i} \eta^j\, d\mathbf{x} = \frac{\delta_{ij}}{R} \int_{B_R(\mathbf{q})} d\mathbf{x} = \frac{4}{3}\pi R^2 \delta_{ij}. \tag{82}$$

Noting that the functions η^j are odd with respect to a plane through the center of the ball we obtain

$$\begin{aligned}
\oint_{\partial B_R(\mathbf{q})} \eta^i \eta^j \eta^k\, dS &= \int_{B_R(\mathbf{q})} \partial_{x^i} \left(\eta^j \eta^k \right) d\mathbf{x} \\
&= \int_{B_R(\mathbf{q})} \eta^j \partial_{x^i} \eta^k + \partial_{x^i}(\eta^j)\eta^k\, d\mathbf{x} \\
&= \frac{1}{R} \int_{B_R(\mathbf{q})} \eta^j \delta_{ik} + \eta^k \delta_{ij}\, d\mathbf{x} \\
&= \frac{\delta_{ik}}{R} \int_{B_R(\mathbf{q})} \eta^j\, d\mathbf{x} + \frac{\delta_{ij}}{R} \int_{B_R(\mathbf{q})} \eta^k\, d\mathbf{x} \\
&= 0.
\end{aligned} \tag{83}$$

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