Modeling phase change at drop scale with combined effects of temperature and concentration gradients

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Abstract

The aim of this paper is to examine and model the mechanisms that are responsible for evaporation of a drop in a multi-component gaseous environment, in the simultaneous presence of temperature and mass concentration gradients. Phase change of a liquid to vapor may occur following three main mechanisms:

- Evaporation by external heat supply from the gas. Heat release occurs through the liquid /gas interface.
- The evaporation or drying by concentration gradients. The simplest example is that a piece of cloth placed in a stream of dry air.
- Evaporation of a liquid by decompression. This phenomenon is the one that occurs in cavitating and 'flashing' flows. In this context, no external energy supply is required. The energy necessary to the phase change is already contained in the liquid phase, in the form of internal energy.

Vapor condensation is the symmetrical process compared to the first two ones and can thus be treated in the same manner. Therefore we focus on the following mass transfer based on diffusive mechanisms: Heat diffusion and molecular diffusion at the interface. In the proposed approach, we make a significant change compared to models found in the literature:

- The mechanisms of evaporation due to temperature and concentration gradients are considered simultaneously.
- Unlike conventional models that assume drops at saturation temperature, a heating delay is considered.

In order to have an efficient phase change sub-model for multiphase non-equilibrium codes, the subscale model must form and algebraic system and not a differential one. In particular, space numerical resolution must be absent.

Keywords, Two-phase flow, evaporation, heat-mass transfer, gradient concentration,diffusion

1. Basic local equations inside each phase

We consider the presence of a pure gas and a pure liquid on both sides of the interface. Across the interface exchanges of mass, momentum and energy occur. The notation for each phase k are the following: l for the liquid phase and g for the gas phase. The equations of conservation of mass of each chemical species i in the phase k are:

$$\frac{\partial \rho_k Y_{ki}}{\partial t} + \vec{\nabla} \cdot (\rho_k Y_{ki} \vec{u}_k - \rho_k D_{ki} \vec{\nabla} Y_{ki}) = 0$$

Where,

ρ_k represents the density of phase k which may consist of different chemical species in the mixture,

Y_{ki} represents the mass fraction of each chemical species i at the phase k,

$\vec{u}_k$ denotes the velocity vector of phase k,

D_{ki} is the mass diffusion coefficient of each chemical species i in the phase k.

In the description given by the above equation, each phase k represents an ideal multi-component mixture. All components are in the same physical state (liquid or gas) and the mixing is at molecular scale. Consequently, all species i have the same temperature which is that of the phase k.

All chemical species at each phase k are assumed to have the same mass diffusion coefficient, which means that, $D_{ki} = D_{kj} = D_k$.

The equations of conservation of energy of the phase k are:

$$\frac{\partial \rho_k E_k}{\partial t} + \vec{\nabla} \cdot (\rho_k E_k \vec{u}_k + p_k \vec{u}_k + \vec{q}_k) = \overline{\overline{\tau}}_k : \vec{\nabla} \vec{u}_k$$

Where:

E_k represents the total energy of phase k which is defined by $E_k = e_k + \frac{1}{2} \vec{u}_k . \vec{u}_k$, in which,

e_k represents the internal energy of phase k,

$\vec{q}_k$ denotes the heat flux that diffuses at phase k,

Energy production by viscous dissipation is neglected. It means that: $\overline{\overline{\tau}}_k : \nabla \vec{u}_k = 0$.

The flow is assumed to be isobaric (constant pressure through time: $\frac{dp_k}{dt} = 0$). This assumption is realistic since an evaporation front spreads in general at very low speed and the diffusion speed for both heat and mass is quite small (less than mm/s). At both sides of the evaporation front and through it significantly fast acoustic wave propagates (with speed of the order of 1000 m/s). The speed of these waves has the effect to almost instantly equilibrate the pressures that would appear through the evaporation front. Considered the flow as isobaric is a commonly used assumption in combustion theory. This approximation allows avoiding consideration of the equations of motion of each phase. Thus no momentum equation is considered.

Writing the above two equations in the coordinate reference system of the interface (which moves at the speed σ) we will obtain the same system of equations as these equations are Galilean invariant. The only modification appears in the velocity definition that is expressed in the reference frame of the interface. Using the total enthalpy definition $h_k = E_k + \frac{p_k}{\rho_k}$ and substituting in the previous equation we get the following system of governing equations:

$$\frac{\partial \rho_k Y_{ki}}{\partial t} + \vec{\nabla} \cdot (\rho_k Y_{ki} \vec{\hat{u}}_k - \rho_k D_k \vec{\nabla} Y_{ki}) = 0$$

$$\frac{\partial \rho_k E_k}{\partial t} + \vec{\nabla} \cdot (\rho_k h_k \vec{\hat{u}}_k + \vec{q}_k) = 0$$

Where $\vec{\hat{u}}_k = \vec{u}_k - \vec{\sigma}$.

Hereafter the notation ‘ $\hat{}$ ’ will be omitted.

2. Interface jump conditions

We consider the case where a drop of pure liquid is evaporating into air. There are two phases k which are considered and two chemical species: water and air.

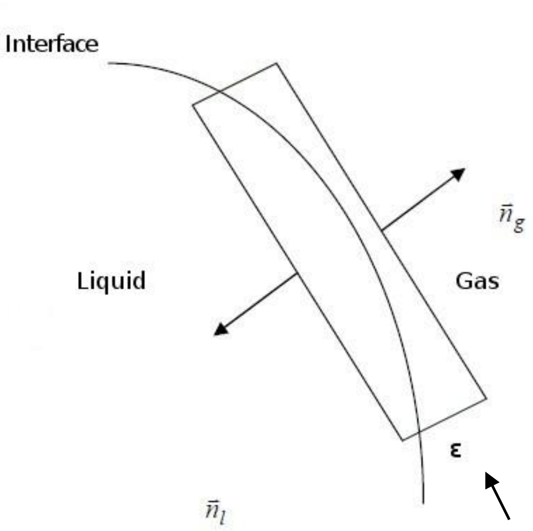
Initial conditions

Inside the drop: $Y_{l,water} = 1$ and $Y_{l,air} = 0$

Outside the drop: $Y_{g,water} = 0$ and $Y_{g,air} = 1$

Through time evolution the concentration of gas varies ($Y_{g,water} \neq 0$ and $Y_{g,air} \neq 1$) but the concentrations in the liquid phase remain invariant.

Consider a finite volume at the interface of the drop as shown in the picture below:



The above equations are integrated in the volume control. As the interface is a discontinuity and the equations are expressed in the front frame of reference, time derivatives of System are dropped.

At each point M (x, y, z) of the volume control, the flow variables have their own value and in particular these variables are discontinuous through the interface except for the pressure that is assumed constant, at least at leading order:

$$\int_V \vec{\nabla} \cdot (\rho Y_i \vec{u} - \rho D \vec{\nabla} Y_i) dV = 0$$

$$\int_V \vec{\nabla} \cdot (\rho h \vec{u} + \vec{q}) dV = 0$$

Using Gauss theorem they become:

$$\int_S (\rho Y_i \vec{u} - \rho D \vec{\nabla} Y_i) \cdot \vec{n} dS = 0$$

$$\int_S (\rho h \vec{u} + \vec{q}) \cdot \vec{n} dS = 0$$

Surface S is composed by a liquid surface S_l and a gas surface S_g as well as ‘side’ surfaces of size ε that tends to zero. Therefore the preceding surface integrals become:

$$\int_{S_l} (\rho_l Y_{li} \vec{u}_l - \rho_l D_l \vec{\nabla} Y_{li}) \cdot \vec{n}_l dS + \int_{S_g} (\rho_g Y_{gi} \vec{u}_g - \rho_g D_g \vec{\nabla} Y_{gi}) \cdot \vec{n}_g dS = 0$$

$$\int_{S_l} (\rho_l h_l \vec{u}_l + \vec{q}_l) \cdot \vec{n}_l dS + \int_{S_g} (\rho_g h_g \vec{u}_g + \vec{q}_g) \cdot \vec{n}_g dS = 0$$

Where:

- $\vec{n}_l$ and $\vec{n}_g$ denote the outward unit normal vectors to the corresponding phases.
- The notation I denotes the interface.

The system of equations thus becomes:

$$\left[(\rho_l Y_{li} \vec{u}_l - \rho_l D_l \vec{\nabla} Y_{li}) \cdot \vec{n}_l + (\rho_g Y_{gi} \vec{u}_g - \rho_g D_g \vec{\nabla} Y_{gi}) \cdot \vec{n}_g \right]_I = 0$$

$$\left[(\rho_l h_l \vec{u}_l + \vec{q}_l) \cdot \vec{n}_l + (\rho_g h_g \vec{u}_g + \vec{q}_g) \cdot \vec{n}_g \right]_I = 0$$

2.1 Examination of the mass jump condition at the interface

We write the mass conservation equation for each species i. Upon summation we get,

$$(\rho_l \vec{u}_l \sum_i Y_{li} - \rho_l D_l \sum_i \vec{\nabla} Y_{li}) \cdot \vec{n}_l + (\rho_g \vec{u}_g \sum_i Y_{gi} - \rho_g D_g \sum_i \vec{\nabla} Y_{gi}) \cdot \vec{n}_g = 0$$

which can be simplified as,

$$\sum_k \rho_k \vec{u}_k \vec{n}_k = 0$$

or in a more convenient form as,

$$\dot{m}_l + \dot{m}_g = 0$$

Using this last relation, the equation of mass conservation becomes for each chemical species i,

$$\dot{m}_l Y_{li} - \rho_l D_l \nabla Y_{li} \cdot \vec{n}_l + \dot{m}_g Y_{gi} - \rho_g D_g \nabla Y_{gi} \cdot \vec{n}_g = 0$$

Considering Fick's first law of diffusion,

$$J_{ki} = -\rho_k D_k \nabla Y_{ki}$$

simplifications appear,

$$\dot{m}_l Y_{li} + J_{li} . \vec{n}_l + \dot{m}_g Y_{gi} + J_{gi} . \vec{n}_g = 0$$

Since $\sum_i Y_{ki} = 1$ we get $\vec{\nabla} \sum_i Y_{ki} = 0$ which asserts $\sum_i \vec{J}_{ki} = 0$.

So both gas and liquid phase have a molecular diffusion for each chemical species which in total is zero.

It is worth to mention that the above simplified expressions are differential equations as gradients are present in the Fick's law. In order to transform these ODEs to an algebraic system (without gradients) we introduce mass exchange coefficients:

$$\vec{J}_{ki} = \rho_k H_{Mk} \left(Y_{ki,I} - Y_{ki,\infty} \right) \vec{n}_k$$

Where:

$Y_{ki,I}$ represents the concentration of species i of phase k at the interface,

$Y_{ki,\infty}$ represents the concentration of species i of phase k far away form the interface,

H_{Mk} denotes the coefficient that represents mass exchange. This coefficient will be expressed with the help of Sherwood number correlations as detailed later.

The index k in the above relationship indicates the mass exchange coefficients H_{Mk} on both sides of the interface. In the present work we may assume that only one common exchange coefficient for the gas phase is employed. Consequently, the gas phase index is dropped $H_{Mg} = H_M$.

Estimation of the diffusion mass exchange coefficient

The mass exchange coefficient between the gas phase and the interface is expressed from the Sherwood number definition,

$$Sh = \frac{H_M d}{D}$$

where d is a characteristic length of the problem (the drop diameter for example). Sherwood number correlations are deduced from Nusselt number ones. Nusselt number correlations are of the form,

$$Nu = a + b \Pr^c \mathrm{Re}^d$$

Where,

- Parameters a, b, c and d are parameters given by experiments for isolated drops as well as drop clouds.
- $\Pr$ is Prandtl number (with $\Pr = \frac{\mu C_P}{\lambda}$, μ the dynamic viscosity, C_P the heat capacity factor, and λ the thermal conductivity). These quantities are specific to each fluid.
- Re is the Reynolds number $\mathrm{Re} = \frac{\rho d \Delta u}{\mu}$, where Δu represents the velocity slip between the phases, determined on the basis of a two-phase flow model. Such a model consists of a system of partial differential equations describing the mean evolution of the two-phase mixture (for example, see Saurel and Le Metayer, 2001)

There are plenty of correlations to calculate Nusselt number for instance for flows around drops, cylinders, plates and more sophisticated geometries. This means that all of parameters a, b, c and d are determined for configurations of interest regarding the Nusselt number. Then the same parameters are applied to the Sh correlation. The Sherwood number is then determined by the following formula:

$$Sh = a + bSc^{c}\,\mathrm{Re}^{d}$$

Where Sc is the Schmidt number $Sc = \dfrac{\mu}{\rho D}$ characteristic of a given fluid.

The system of mass equations can be summarized as follows:

$$\dot{m}_l Y_{li,I} + J_{li}\cdot\vec{n}_l + \dot{m}_g Y_{gi,I} + J_{gi}\cdot\vec{n}_g = 0$$

$$J_{ki} = \rho_k H_{Mk}(Y_{ki,I} - Y_{ki,\infty})\vec{n}_k$$

$$Sh_k = \frac{H_{Mk} d}{D_k}$$

$$Sh_k = a_k + b_k Sc_k^{c_k}\,\mathrm{Re}_k^{d_k}$$

Including the constraint: $\dot{m}_l + \dot{m}_g = 0$

Using the mass exchange coefficient the first equation becomes the following algebraic equation:

$$\dot{m}_l Y_{li,I} + \rho_l H_{Ml}(Y_{li,I} - Y_{li,\infty}) + \dot{m}_g Y_{gi,I} + \rho_g H_{Mg}(Y_{gi,I} - Y_{gi,\infty}) = 0$$

The quantities $\rho_l, \rho_g, \mathrm{H}_M, \mathrm{H}_{Mg}, Y_{li,\infty}, Y_{gi,\infty}$ are determined from the 'average two-phase model' and Sherwood correlations. It thus remain 4 unknowns: $Y_{li,I} Y_{gi,I}, \dot{m}_l$ and $\dot{m}_g$.

Example: Consider a drop with initially only water at one side of the interface and on the other side of the interface air and water vapor. The initial data are:

- At the liquid part: $Y_{l,water} = 1, \mathrm{Y}_{l,air} = 0$
- At the interface part: $Y_{l,water,I} = 1, \mathrm{Y}_{l,air,I} = 0$
- At the gas part: $Y_{g,water} \neq 1, \mathrm{Y}_{\mathrm{g},air} \neq 0$
- At the far away part: $Y_{l,water,\infty} = 1, \mathrm{Y}_{l,air,\infty} = 0$

From the concentrations at the liquid part we get: $Y_{li,I} - Y_{li,\infty} = 0$ so the equation for mass exchange can be written for water and air respectively as below:

$$\dot{m}_l + \dot{m}_g Y_{g,water,I} + \rho_g H_{Mg}(Y_{g,water,I} - Y_{g,water,\infty}) = 0$$

$$\dot{m}_g Y_{g,air,I} + \rho_g H_{Mg}(Y_{g,air,I} - Y_{g,air,\infty}) = 0$$

Summing these two equations, the mass conservation at the interface is satisfied, meaning that, $\dot{m}_l + \dot{m}_g = 0$. Therefore the preceding system can be considered as:

$$\dot{m}_l + \dot{m}_g Y_{g,water,I} + \rho_g H_{Mg}(Y_{g,water,I} - Y_{g,water,\infty}) = 0$$

$$\dot{m}_l + \dot{m}_g = 0$$

Simplifying again gives the following expression:

$$\dot{m}_g = \frac{\rho_g H_{Mg}(Y_{g,water,I} - Y_{g,water,\infty})}{1 - Y_{g,water,I}}$$

This equation expresses the gas mass flow rate emitted by a liquid surface under the sole effect of the molecular mass diffusion. Such a situation occurs when the temperature of the liquid and gas are in equilibrium. We may observe this type of situation when drying clothes in a stream of dry air ($Y_{g,water,I} > 0, Y_{g,water,\infty} = 0$). In this case, $\dot{m}_g > 0$ meaning that the gas mass increases while the cloth loses liquid. Conversely, if the air is humid and the cloth is dry then $\dot{m}_g < 0$. Thereafter we consider energy aspects that will be important when a thermal disequilibrium is present.

2.2 Examination of the interface energy jump relation

The corresponding equation has already been determined in the above simplified system of equations,

$$(\rho_l h_l \vec{u}_l + \vec{q}_l) \cdot \vec{n}_l + (\rho_g h_g \vec{u}_g + \vec{q}_g) \cdot \vec{n}_g = 0\,,$$

where the heat flux is given by the sum of Fourier and energy transport by mass diffusion terms,

$$\vec{q}_k = -\lambda_k \vec{\nabla} T_k - \rho_k D_k \sum_i h_{ki} \vec{\nabla} Y_{ki}$$

The mixture enthalpy is defined by $h_k = \sum_i Y_{ki} h_{ki}$.

With the help of the mass flow rate definition, it becomes:

$$\dot{m}_l h_l + \vec{q}_l \cdot \vec{n}_l + \dot{m}_g h_g + \vec{q}_g \cdot \vec{n}_g = 0\,.$$

Inserting the heat flux definition we have,

$$\dot{m}_l \sum_i Y_{li} h_{li} - \rho_l D_l \sum_i h_{li} \overrightarrow{\nabla Y}_{li} \cdot \vec{n}_l - \lambda_l \overrightarrow{\nabla T}_l \cdot \vec{n}_l + \dot{m}_g \sum_i Y_{gi} h_{gi} - \rho_g D_g \sum_i h_{gi} \overrightarrow{\nabla Y}_{gi} \cdot \vec{n}_g - \lambda_g \overrightarrow{\nabla T}_g \cdot \vec{n}_g = 0$$

or,

$$\sum_i h_{li} (\dot{m}_l Y_{li} - \rho_l D_l \overrightarrow{\nabla Y}_{li} \cdot \vec{n}_l) - \lambda_l \overrightarrow{\nabla T}_l \cdot \vec{n}_l + \sum_i h_{gi} (\dot{m}_g Y_{gi} - \rho_g D_g \overrightarrow{\nabla Y}_{gi} \cdot \vec{n}_g) - \lambda_g \overrightarrow{\nabla T}_g \cdot \vec{n}_g = 0$$

From the mass conservation at the interface for each species i :

$$\dot{m}_l Y_{li} - \rho_l D_l \overrightarrow{\nabla Y}_{li} \cdot \vec{n}_l + \dot{m}_g Y_{gi} - \rho_g D_g \overrightarrow{\nabla Y}_{gi} \cdot \vec{n}_g = 0$$

The energy equation becomes,

$$\sum_i (h_{li} - h_{gi})(\dot{m}_l Y_{li} - \rho_l D_l \overrightarrow{\nabla Y}_{li} \cdot \vec{n}_l) - \lambda_l \overrightarrow{\nabla T}_l \cdot \vec{n}_l - \lambda_g \overrightarrow{\nabla T}_g \cdot \vec{n}_g = 0$$

With the help of the Fourier law,

$$\vec{q}_{ck} = -\lambda_k \nabla T_k$$

As done previously with mass exchange, the Fourier law is replaced by a heat exchange correlation. Indeed,

$$\vec{q}_{ck} \cdot \vec{n}_k = -\lambda_k \overrightarrow{\nabla T}_k \cdot \vec{n}_k = H_{Tk} \left(T_I - T_{k,\infty} \right)$$

Where:

- H_{Tk} represents the heat exchange coefficient. This coefficient is expressed with the Nusselt number correlations.
- T_I is the interface temperature.
- $T_{k,\infty}$ is the temperature of phase k far away of the interface.

The interface energy condition now becomes:

$$\sum_i (h_{li} - h_{gi})(\dot{m}_l Y_{li} - \rho_l H_{Ml} (Y_{li,I} - Y_{li,\infty})) + H_{Tl} (T_I - T_{l,\infty}) + H_{Tg} (T_I - T_{g,\infty}) = 0$$

Example: Reconsidering the previous example with a liquid made of pure water the term where H_{Ml} is present vanishes. The above relationship becomes:

$$(h_{l,water} - h_{g,water}) \dot{m}_l + H_{Tl} (T_I - T_{l,\infty}) + H_{Tg} (T_I - T_{g,\infty}) = 0$$

Therefore, a second expression for the mass flow rate appears:

$$\dot{m}_l = \frac{H_{Tl} (T_I - T_{l,\infty}) + H_{Tg} (T_I - T_{g,\infty})}{h_{g,water} - h_{l,water}}$$

As the evaporation process is isobaric, the enthalpy difference corresponds to the latent heat of vaporization:

$$h_{g,water} - h_{l,water} = L_{v,water}(P)$$

Using the interface mass condition the gas mass flow rate reads:

$$\dot{m}_g = \frac{H_{Tl}(T_{l,\infty} - T_I) + H_{Tg}(T_{g,\infty} - T_I)}{L_{v,water}(P)}$$

This relationship can be used to determine the mass flow rate when the effects of concentration gradients are absent. This situation corresponds to the case of a drop of liquid placed in steam-only gas environment. In this case the interface mass condition $(\dot{m}_l + \dot{m}_g = 0)$ is automatically satisfied.

When the concentration gradients are present they must satisfy the interface condition for each gas species together with the interface energy condition which complicates the determination of the solution. Note also that the interface energy condition requires the knowledge of H_{Tl} and the interface temperature T_I.

Limit case 1: Let us consider a cold drop in a warm gas (steam only) environment (superheated steam). The temperature of the drop increases and after some time reaches the saturation temperature $T_{sat}(P)$. At this moment the conditions are: $T_{l,\infty} = T_I = T_{sat}(P)$.

The drop then continues evaporation at a rate controlled by the above relation eliminating the term of H_{Tl}:

$$\dot{m}_g = \frac{H_{Tg}(T_{g,\infty} - T_{sat}(P))}{L_{v,water}(P)}$$

Limit case 2: Let us now consider a drop and its surrounding vapor under rapid pressure drop. In this expansion process the temperature within the liquid can exceed the interface temperature. But considering local thermodynamic equilibrium at the interface, its temperature is still given by:

$$T_I = T_{sat}(P)$$

In such situation, $T_{l,\infty} \geq T_I$ and we assume a uniform temperature profile inside the drop. In such a process, the dominant term is $H_{Tl}(T_{l,\infty} - T_I)$. The internal energy stored in the liquid is responsible for its self-vaporization. This occurs for example in flashing and cavitating flows.

3. Closure relations

Let us consider the evaporation model in the special case where only two chemical species are present. The system to consider is made of the interface mass and energy jump conditions. So both relationships for gas mass flow rate have to be considered:

$$\dot{m}_g = \frac{\rho_g H_{Mg} (Y_{g,water,I} - Y_{g,water,\infty})}{1 - Y_{g,water,I}}$$

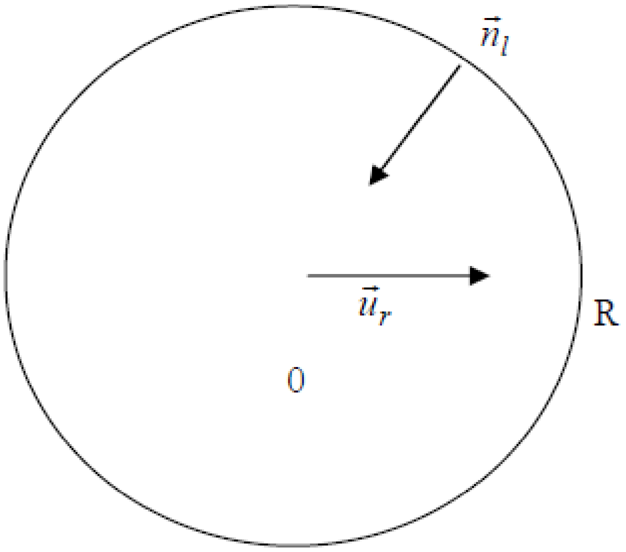
$$\dot{m}_g = \frac{H_{Tl} (T_{l,\infty} - T_I) + H_{Tg} (T_{g,\infty} - T_I)}{L_v (P)}$$

This system involves 4 unknowns: $\dot{m}_g, Y_{g,water,I}, \mathrm{T}_I, H_{Tl}$. Indeed, the other variables (such as for example gas-interface exchanges correlation or the pressure P) are given by appropriate correlations and flow variables of the two-phase mixture. These last ones are determined by averaged equations of the two-phase flow model. Such system corresponds to a set of partial differential equations for which the present mass transfer model is a sub-model.

Heat transfer coefficient H_{Tl} inside the drop is unknown but the gas coefficient H_{Tg} is easily determined from correlations based on the Nusselt number. This is because the temperature measurement within a drop is nothing easy. Moreover, the field of the internal flow in the droplet cannot be quantified from the information provided by the macroscopic two-phase model. To our knowledge, no effective correlation is available for the determination of this transfer coefficient. This is why conventional models in principle not consider heating stage of drops before reaching the saturation temperature. Next we address an approximate method to estimate of this heat exchange coefficient. A relation for the determination of the vapor water concentration at the interface $Y_{g,water,I}$ is developed as well.

3.1 Determination of the liquid-interface heat exchange coefficient

Let us consider a spherical drop as shown on the following picture:



Due to internal convection inside the drop, surface tension at the interface and heat exchange with the gas it is not possible to address internal temperature profile inside the drop in agreement with fundamental equations of this complex flow. We thus consider a temperature profile that fulfils the basic constraints which are undoubted:

- $\left.\dfrac{\partial T}{\partial r}\right|_{r=0} = 0$ symmetry condition,
- $T_{r=R} = T_I$ condition at the interface,
- $\overline{T_l} = \dfrac{1}{V}\int_V T(r)\,dV$ mean temperature definition.

The last relationship holds since the macroscopic two-phase flow model provides the total energy average for a given phase and consequently it's average temperature. We then have three conditions that we can use to determine the algebraic form of the temperature field. This profile may involve three parameters. We will then choose the simplest profile involving only three parameters, i.e. a parabolic profile:

$$T(r) = ar^2 + br + c$$

After taking the derivative $\dfrac{\partial T}{\partial r} = 2ar + b$ and applying the symmetry condition $\left.\dfrac{\partial T}{\partial r}\right|_{r=0} = 0$ we shall get $b = 0$.

The second condition at the interface reads, $T_I = aR^2 + c$.

Integrating the temperature profile,

$$\overline{T_l} = \frac{3}{R^3}\int_0^R T(r)r^2 dr\ ,$$

the following result is obtained,

$$\overline{T_l} = \frac{3aR^2}{5} + c\ .$$

After integrating and eliminating the constant c we get: $T_I - \overline{T_l} = \dfrac{2aR^2}{5}$

Therefore, $a = \dfrac{5\left(T_I - \overline{T_l}\right)}{2R^2}$.

The temperature profile thus reads,

$$T(r) = \frac{5(T_I - \overline{T_l})}{2}\left(\frac{r}{R}\right)^2 + \overline{T_l} - \frac{3aR^2}{5}$$

The heat flux at the interface is defined by,

$$\vec{q}_{l,I} = -\lambda_l \left.\frac{\partial T_l}{\partial r}\right|_{r=R} \vec{u}_r$$

Where λ_l is the thermal conductivity. The heat exchange coefficient is given by:

$$\vec{q}_{l,I} \cdot \vec{n}_l = H_{Tl}(T_I - T_{l,\infty})$$

Since $\vec{n}_l = -\vec{u}_r$, we get: $\lambda_l \frac{5(T_I - \overline{T_l})}{R} = H_{Tl}(T_I - T_{l,\infty})$.

Assuming that $\overline{T_l} = T_{l,\infty}$ the desirable relationship is obtained:

$$H_{Tl} = \frac{5\lambda_l}{R}$$

This solution guarantees the energy conservation at the whole drop. It also corresponds to an internal Nusselt number of 10.

3.2 Thermodynamic relationships at the interface

The last step is to determine the concentration of the vapor water at the interface $Y_{g,water,I}$ and the interface temperature T_I . We aim to find an algebraic equation which links these two variables.

The interface is in thermodynamic equilibrium which means:

a) $T_{g,I} = T_{l,I} = T_I$ (thermal equilibrium)

b) $P_{g,I} = P_{1,I} = P_I$ (mechanical equilibrium)

c) $\mu_{g,I} = \mu_{1,I}$ (chemical equilibrium - see Appendix A)

These three conditions result in the partial pressure of vapor at the drop surface that it is equal to the saturation pressure at the outlet interface temperature:

$$P_{g,\text{water},I} = P_{sat}(T_I)$$

From the Dalton law for ideal gases the total pressure of the gas mixture is equal to the sum of the partial pressures of individual gas species. For the vapor,

$$P_{g,\text{water},I} V = n_{g,water,I} R T_I$$

The equation of state expressed at the interface for the gas mixture gives:

$$PV = \sum_i n_{g,\mathrm{i},I} R T_I$$

Using the mole fraction definition $x_i = \frac{n_i}{\sum_i n_i}$ we get:

$$x_{g,\mathrm{water},I} = \frac{P_{g,\mathrm{water},I}}{P} = \frac{P_{sat}(T_I)}{P}$$

In order to convert the mole fractions to mass fractions we apply the following relation: $Y_i = \frac{n_i M_i}{\sum_i n_i M_i}$,

Where, M_i is the molecular mass of species i. Moreover the mixture molar mass is defined by: $\hat{M} = \frac{\sum_i n_i M_i}{\sum_i n_i}$.

With this definition since $\hat{M} \sum_i n_i = \sum_i n_i M_i$ we obtain: $Y_i = x_i \frac{M_i}{\hat{M}}$

Which leads to the following formula, $Y_i = \frac{M_i}{\hat{M}} \frac{P_{sat}(T_I)}{P}$.

Substitution of the expression for $x_{g,\mathrm{water},I}$ gives,

$$Y_{g,\mathrm{water},I} = \frac{M_{water}}{\hat{M}} \frac{P_{sat}(T_I)}{P}$$

3.3 System of governing equations

Two chemical species

The relationships that govern the evaporation rate when only two chemical species are present (water and air for example) are the following:

$$\dot{m}_g = \frac{\rho_g H_{Mg} (Y_{g,\mathrm{water},I} - Y_{g,\mathrm{water},\infty})}{1 - Y_{g,\mathrm{water},I}} \tag{A}$$

$$\dot{m}_g = \frac{H_{Tl}(T_{l,\infty} - T_I) + H_{Tg}(T_{g,\infty} - T_I)}{L_{v,\mathrm{water}}(P)} \tag{B}$$

$$Y_{g,\mathrm{water},I} = \frac{M_{water}}{\hat{M}} \frac{P_{sat,\mathrm{water}}(T_I)}{P} \tag{C}$$

Since the heat exchange coefficient H_{Tl} was previously determined and the relation $P_{sat,\mathrm{water}}(T_I)$ is provided by the phase diagram of the fluid in consideration, this system comprises only 3 unknowns: $\dot{m}_g, Y_{g,\mathrm{water},I}$ and T_I. The mass fraction of the air which is also involved in the calculation of the gas mixture molar mass is obtained from:

$$Y_{g,\mathrm{water},I} + Y_{g,\mathrm{air},I} = 1 .$$

This system however is a highly nonlinear and specific solution procedure need to be implemented. As an initial option the following procedure is proposed:

i) Start from an initial estimate of the interface temperature T_I for $\dot{m}_g = 0$.

Then from equation (B): $T_I = \dfrac{H_{Tl}T_{l,\infty} + H_{Tg}T_{g,\infty}}{H_{Tl} + H_{Tg}}$

ii) Calculate $Y_{g,\mathrm{water},I}$ from (C) (must always lie inside the interval of $[0,1]$

iii) Calculate $\dot{m}_g$ from (A)

iv) Calculate the new T_I from (B): $T_I = \dfrac{H_{Tl}T_{l,\infty} + H_{Tg}T_{g,\infty} - \dot{m}_g L_{v,\mathrm{water}}(P)}{H_{Tl} + H_{Tg}}$

Steps ii)-iv) are repeated until two values of T_I merge. This procedure will work when the initial estimate is close to the desired value, ie at very low flow rates. In highly dynamic conditions and in the presence of large differences in concentration and temperature an algorithm of Newton type will be required.

Limit case – Water drop in its vapor

When the gas contains only vapor, we have: $Y_{g,\mathrm{water},I} = Y_{g,\mathrm{water},\infty} = 1$ and relation (A) is inappropriate.

For $P = P_{sat,\mathrm{water}}(T_I)$ or if $T_I = T_{sat}(P)$ in (C) we get obviously: $Y_{g,water,I} = 1$

The mass flow is thus obtained directly from the energy balance (B). The heating step of the drop is nevertheless taken into account. Assuming further that the temperature of the drop is uniform, so that heating is no longer possible $(T_{1,\infty} = T_I)$ the flow rate is obtained by:

$$\dot{m}_g = \frac{H_{Tg}(T_{g,\infty} - T_{sat,\text{water}}(P))}{L_{v,\text{water}}(P)}$$

Generalization of the model

The model can be generalized to the case where the system involves more than two species. A typical example is those of liquid fuel drop initially placed in the air. The evaporation produces a mixture of two species, air and liquid vapor. Then, if combustion occurs a third component appears. This third component may be itself multi-constituent, with some species possibly already present in the air. In these cases all changes of these components need consideration.

Two cases are to be considered:

- The combustion product gas mixture is composed solely of new chemical species. This depends on the combustion chemical reaction. In this case, this gas mixture can be treated as a third chemical species.

- Otherwise, some of the chemical species of combustion products are already present. In that instance all species concentration need determination and the system is obviously complicated.

The following thermodynamic relationship determines the concentration of the gas species at the evaporating side of the interface:

$$Y_{g,ev,I} = \frac{M_{ev}}{\hat{M}} \frac{P_{sat,ev}(T_I)}{P}$$

Where the index ‘ev’ stands for evaporating species. The mass balance of the various species read,

$$\dot{m}_l Y_{l,i,I} + \dot{m}_g Y_{g,i,I} + \rho_g H_{Mg}(Y_{g,i,I} - Y_{g,i,\infty}) = 0 \quad \forall i$$

The effects of molecular diffusion in the liquid phase have been omitted.
In the particular case where the liquid consists of a single species:

$$Y_{l,ev,I} = 1 \text{ and } Y_{l,i,I} = 0 \quad \forall i \neq ev .$$

The above balance equation can be written as,

$$\dot{m}_l + \dot{m}_g Y_{g,ev,I} + \rho_g H_{Mg}(Y_{g,ev,I} - Y_{g,ev,\infty}) = 0 ,$$

$$\dot{m}_g Y_{g,i,I} + \rho_g H_{Mg}(Y_{g,i,I} - Y_{g,i,\infty}) = 0 \qquad \forall i \neq ev .$$

The first of these equations provides the mass flow rate:

$$\dot{m}_g = \frac{\rho_g H_{Mg}(Y_{g,ev,I} - Y_{g,ev,\infty})}{1 - Y_{g,ev,I}}$$

The other equations provide the concentrations of the other constituents at the interface:

$$Y_{g,i,I} = \frac{\rho_g H_{Mg} Y_{g,i,\infty}}{\dot{m}_g + \rho_g H_{Mg}} \quad \forall i \neq ev$$

In the case where the liquid is constituted of only the evaporating species the condition of interface energy is unchanged compared to the preceding case. It is used for the calculation of T_I :

$$T_I = \frac{H_{Tl} T_{l,\infty} + H_{Tg} T_{g,\infty} - \dot{m}_g L_{v,ev}(P)}{H_{Tl} + H_{Tg}}$$

This system involves N species, one of them corresponding to the evaporating species and N + 2 unknowns, the two additional unknowns being $\dot{m}_g$ and T_I . The system above contains N+1 equation. The last equation is provided by,

$$Y_{g,water,I} = \frac{M_{water}}{\hat{M}} \frac{P_{sat,water}(T_I)}{P}.$$

The next step consists of the introduction of this submodel in the macroscopic multiphase flow one. This step is the subject of the next section (or forthcoming work).

Numerical method for solving the sub-model

As soon as the physical modelling is completed we have defined the system of the governing equations we must proceed to the numerics. The target is to develop an efficient, robust and reliable algorithm for the solution of the algebraic equations. Our strategy is to combine the equations to find a nonlinear function of a single variable to be solved. Physical constraints that should be satisfied are also used to test and specify the best numerical method as far the three factors mentioned above. First we apply some computations to transform mathematical relations to a more convenient form:

Since right hand sides of relations (A), (B) so these can be written as:

$$\frac{H_{Tl}(T_{l,\infty} - T_I) + H_{Tg}(T_{g,\infty} - T_I)}{L_{v,eau}(T_I)} = \frac{\rho_g H_{Mg}(Y_{g,eau,I} - Y_{g,eau,\infty})}{1 - Y_{g,eau,I}}$$

We get the relation of temperature as a function of mass fraction,

$$T_I(Y_{g,water,I}) = \left(\frac{H_{Tl} T_{l,\infty} + H_{Tg} T_{g,\infty}}{H_{Tl} + H_{Tg}} \right) - \frac{L_{v,water}(T_I)}{H_{Tl} + H_{Tg}} \frac{\rho_g H_{Mg}(Y_{g,water,I} - Y_{g,water,\infty})}{1 - Y_{g,water,I}}$$

From relation (C) solving for pressure gives,

$$P_{sat,water}(T_I) = \frac{\hat{M}}{M_{water}} P\, Y_{g,water,I}$$

Combing these last two we get,

$$P_{sat}(T_I(Y_{g,water,I})) = P_{sat}\left\{ \left(\frac{H_{Tl}T_{l,\infty} + H_{Tg}T_{g,\infty}}{H_{Tl} + H_{Tg}} \right) - \frac{L_{v,water}(T_I)}{H_{Tl} + H_{Tg}} \frac{\rho_g H_{Mg}(Y_{g,water,I} - Y_{g,water,\infty})}{1 - Y_{g,water,I}} \right\}$$

Now since, $P_{sat,water}(T_I) = \frac{\hat{M}}{M_{water}} P\, Y_{g,water,I}$ we get,

$$f(Y_{g,water,I}) = P_{sat}\left\{ \left(\frac{H_{Tl}T_{l,\infty} + H_{Tg}T_{g,\infty}}{H_{Tl} + H_{Tg}} \right) - \frac{L_{v,water}(T_I)}{H_{Tl} + H_{Tg}} \frac{\rho_g H_{Mg}(Y_{g,water,I} - Y_{g,water,\infty})}{1 - Y_{g,water,I}} \right\} - \frac{\hat{M}(Y_{g,water,I})}{M_{water}} P\, Y_{g,water,I} = 0$$

For a given temperature T_I, function f depends only on mass fraction $Y_{g,water,I}$.This equation is supplemented with both mass fraction and temperature constraints. This means f is valid only for certain values of these variables. These bounds must be primary determined.

So, the equations to zero are,

$$T_I(Y_{g,water,I}) = \left(\frac{H_{Tl}T_{l,\infty} + H_{Tg}T_{g,\infty}}{H_{Tl} + H_{Tg}} \right) - \frac{L_{v,water}(T_I)}{H_{Tl} + H_{Tg}} \frac{\rho_g H_{Mg}(Y_{g,water,I} - Y_{g,water,\infty})}{1 - Y_{g,water,I}}$$

Or more explicit,

$$\left(\frac{H_{Tl}T_{l,\infty} + H_{Tg}T_{g,\infty}}{H_{Tl} + H_{Tg}} \right) - \frac{L_{v,water}(T_I)}{H_{Tl} + H_{Tg}} \frac{\rho_g H_{Mg}(Y_{g,water,I} - Y_{g,water,\infty})}{1 - Y_{g,water,I}} - T_I = 0$$

And,

$$f(Y_{g,water,I}) = P_{sat}\left\{ \left(\frac{H_{Tl}T_{l,\infty} + H_{Tg}T_{g,\infty}}{H_{Tl} + H_{Tg}} \right) - \frac{L_{v,water}(T_I)}{H_{Tl} + H_{Tg}} \frac{\rho_g H_{Mg}(Y_{g,water,I} - Y_{g,water,\infty})}{1 - Y_{g,water,I}} \right\} - \frac{\hat{M}(Y_{g,water,I})}{M_{water}} P\, Y_{g,water,I} = 0$$

for a given range of $Y_{g,water,I}$ and T_I.

The method initially assumes an arbitrary value for $L_{v,water}$ which corresponds to an initial guess for temperature. Thus,

$$T_I(Y_{g,water,I}) = \left(\frac{H_{Tl}T_{l,\infty} + H_{Tg}T_{g,\infty}}{H_{Tl} + H_{Tg}} \right) - \frac{L_{v,water}}{H_{Tl} + H_{Tg}} \frac{\rho_g H_{Mg}(Y_{g,water,I} - Y_{g,water,\infty})}{1 - Y_{g,water,I}}$$

We now have to determine the existence bounds for $Y_{g,water,I}$. We denote this initial guess for T_I (which may varies with the actual temperature) with T^* to distinguish it from the same expression than uses the exact latent heat,

$$T^* = \left(\frac{H_{Tl}T_{l,\infty} + H_{Tg}T_{g,\infty}}{H_{Tl} + H_{Tg}}\right) - \frac{L_{v,water}}{H_{Tl} + H_{Tg}} \frac{\rho_g H_{Mg}(Y_{g,water,I} - Y_{g,water,\infty})}{1 - Y_{g,water,I}}$$

T^* will have a range of values from a minimum value $T_{low} = 0K$ (since negative temperature is not acceptable for saturation pressure calculation) to a maximum $T_{up} = T_{crit}$ the fluid critical temperature which is also used as a physical constraint.

Thus,

$$Y_{g,water,I} = \frac{Y_{g,water,\infty} + \left(\dfrac{\dfrac{H_{Tl}T_{l,\infty} + H_{Tg}T_{g,\infty}}{H_{Tl} + H_{Tg}} - T^*}{\dfrac{\rho_g H_{Mg} L_{v,water}}{H_{Tl} + H_{Tg}}}\right)}{1 + \left(\dfrac{\dfrac{H_{Tl}T_{l,\infty} + H_{Tg}T_{g,\infty}}{H_{Tl} + H_{Tg}} - T^*}{\dfrac{\rho_g H_{Mg} L_{v,water}}{H_{Tl} + H_{Tg}}}\right)}$$

Therefore, setting $T_{low} = 0K$ the lower fraction bound is:

$$Y_{g,water,I,low} = \frac{Y_{g,water,\infty} + \left(\dfrac{H_{Tl}T_{l,\infty} + H_{Tg}T_{g,\infty}}{\rho_g H_{Mg} L_{v,water}}\right)}{1 + \left(\dfrac{H_{Tl}T_{l,\infty} + H_{Tg}T_{g,\infty}}{\rho_g H_{Mg} L_{v,water}}\right)}$$

This bound is obviously positive.

The upper bound is,

$$Y_{g,water,I,up} = \frac{Y_{g,water,\infty} + \left(\dfrac{\dfrac{H_{Tl}T_{l,\infty} + H_{Tg}T_{g,\infty}}{H_{Tl} + H_{Tg}} - T_{up}}{\dfrac{\rho_g H_{Mg} L_{v,water}}{H_{Tl} + H_{Tg}}} \right)}{1 + \left(\dfrac{\dfrac{H_{Tl}T_{l,\infty} + H_{Tg}T_{g,\infty}}{H_{Tl} + H_{Tg}} - T_{up}}{\dfrac{\rho_g H_{Mg} L_{v,water}}{H_{Tl} + H_{Tg}}} \right)}$$

This bound has to be less than 1. This is not obvious as for the moment, T_{up} is more or less arbitrary.

Therefore, in order that temperature T_I stays positive, $Y_{g,water,I}$ must belong to the interval:

$$Y_{g,water,I,low} < Y_{g,water,I} < Y_{g,water,I,up}$$

The precise value of $Y_{g,water,I}$ is then determined by solving,

$$f\left(Y_{g,water,I}\right) = P_{sat}\left\{ \left(\frac{H_{Tl}T_{l,\infty} + H_{Tg}T_{g,\infty}}{H_{Tl} + H_{Tg}} \right) - \frac{L_{v,water}(T_I)}{H_{Tl} + H_{Tg}} \frac{\rho_g H_{Mg}\left(Y_{g,water,I} - Y_{g,water,\infty}\right)}{1 - Y_{g,water,I}} \right\} - \frac{\hat{M}\left(Y_{g,water,I}\right)}{M_{water}} P\ Y_{g,water,I} = 0$$

When $Y_{g,water,I}$ is determined, T_I is computed by,

$$T_I = T^*\left(Y_{g,water,I}\right) = \left(\frac{H_{Tl}T_{l,\infty} + H_{Tg}T_{g,\infty}}{H_{Tl} + H_{Tg}} \right) - \frac{L_{v,water}}{H_{Tl} + H_{Tg}} \frac{\rho_g H_{Mg}\left(Y_{g,water,I} - Y_{g,water,\infty}\right)}{1 - Y_{g,water,I}}$$

This (new) T_I is used to compute $L_{v,water}(T_I)$ that is used for the next time step in the same computational cell. Latent heat is an important factor that can effect computations and is updated at every new temperature.

The steps for the solution of the sub-model:

1. Define minimum and maximum temperature
2. Define desired accuracy of solution
3. Make an initial guess for $L_{v,water}(T^*_I)$ for an initial T^*_I
4. Fix the initial bounds for Y_{gwI}

5. Determine $Y_{gwI}{}^{*}$ so that $f(Y_{gwI}) = 0$ (or $\left|f(Y_{gwI})\right| \leq 1Pa$). This can be done by dichotomy for example.
6. Compute the new temperature $T^{new} = T^{*}{}_{I}(Y_{gwI})$
7. Check if the difference $T^{new} - T^{*}$ is smaller than the desired accuracy
8. Update $L_{v,water}(T_{I}{}^{new})$ for the new temperature and go to 4.
9. Find the new bounds for Y_{gwI}
10. If temperature convergences then verify that initial expressions (A),(B),(C) are reasonable

Solving the non-linear equation

The last task we have to work on is choosing an appropriate method for solving the non- linear equation $f(Y_{gwI}) = 0$ numerically. Starting from some approximate trial solution, an algorithm will improve the solution until the desired convergence criterion is satisfied. Zero finding depends on a good first guess. However it is not the only thing that can affect the solution. An insight analysis of the problem is required to apply or modify a method so that it successfully solves the problem taking in concern all the necessary constraints.

We are always looking to bracket the root by the sign changes of the function. That is the reason that the range of function $f(Y_{gwI})$ is always updated. Solution must be inside this range and a good algorithm should not get outside of this bounds.

The equations we want to solve are approximately like this:

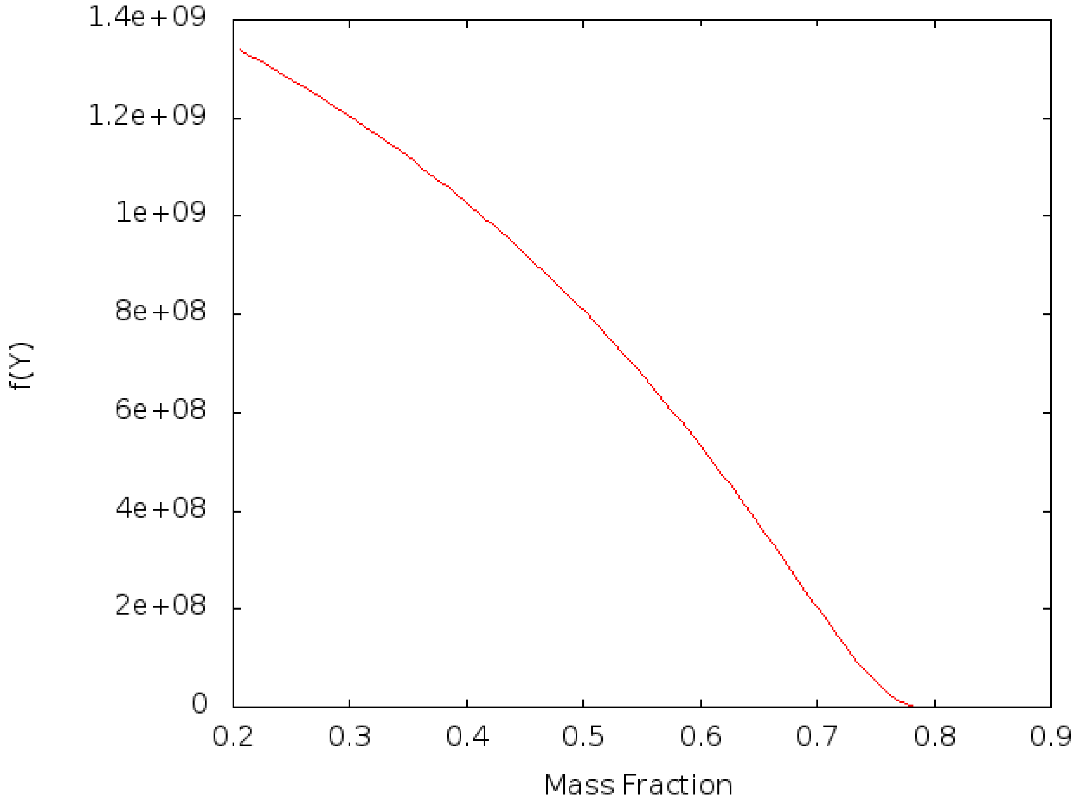


Figure 1. Equation $f(Y_{gwI})$ for constant latent heat, $L_v = 2 \cdot 10^6 J/kg$

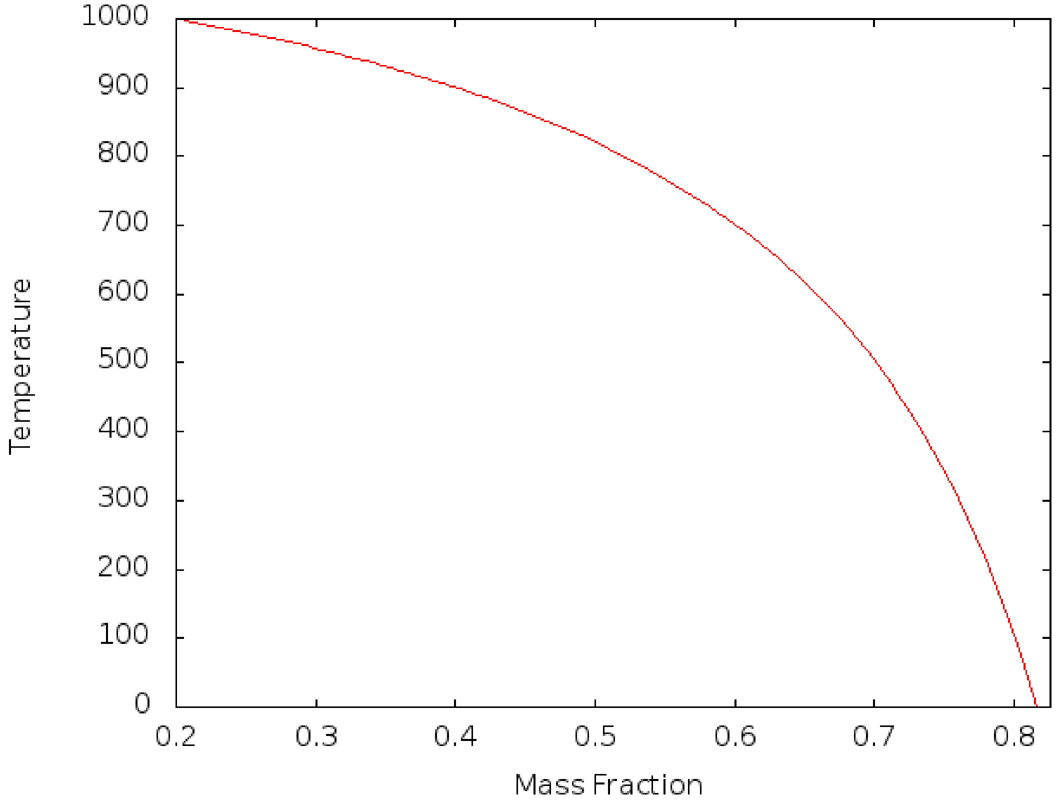


Figure 2. Function $T(Y_{gwI})$ for constant latent heat, $L_v = 2 \cdot 10^6 J/kg$

Dichotomy method

In this method, evaluation of the function is made inside a sub-interval of the bracket that we fix at every iteration. This sub-interval is divided by two at every sign change. This method is successfully applied with a small number of iteration (less than ten).

Let a_n, b_n be the endpoints at the *n*-th iteration (with $a_1 = Y_{gwI}^{min}$ and $b_1 = Y_{gwI}^{max}$) and let r_n be the *n*-th approximate solution. Then r_n is defined by $r_n = \frac{1}{2}(a_n + b_n)$ and the interval now has length equal to $b_n - a_n = \frac{b - a}{2^{n-1}}$.

Secant (False position) method

Again the method is applied at the bracket we fix in order for the function $f(Y_{gwI})$ to be valid. If solution is bracketed between a_n and b_n at the *n*-th iteration, then the new root estimate r_n is,

$$r_n = \frac{b_n f(a_n) - a_n f(b_n)}{f(a_n) - f(b_n)}$$

This method is faster than dichotomy but convergences to solution that lies close to T_{min}.

Chord method

This method does not differ from the previous in only exception: that keeps the most recent of the prior estimates and as in Secant (False Position) method, the function is assumed to be linear close to the solution, so the slope between to estimate points is given by,

$$f'(x_{n-1}) \approx \frac{f(x_{n-1}) - f(x_{n-2})}{x_{n-1} - x_{n-2}}$$

So the new root guess is,

$$x_n = x_{n-1} - \frac{f(x_{n-1})(x_{n-1} - x_{n-2})}{f(x_{n-1}) - f(x_{n-2})}$$

The root does not necessarily remains bracketed or the solution can be slow because of the function's local behaviour. This issue also occurs at Newton's method (where again the solution lies close to T_{min}).

Ridders' method

It is a slightly different from the two others. The root is bracketed between two values and evaluation is done at their midpoint. The new idea here is that it uses an exponential function which turns the residual function into a straight line [4], giving a new guess for the root. It can be superlinear and gives successfully a root. One can use different accuracy levels for the two equations. If the root is bracketed inside two points x_1 and x_2 and $x_3 = \frac{1}{2}(x_1 + x_2)$ is their midpoint, then the new root guess is,

$$x_4 = x_3 + (x_3 - x_1)\frac{\text{sign}\left[f(x_1) - f(x_2)\right]f(x_3)}{\sqrt{f(x_3)^2 - f(x_1)\,f(x_2)}}$$

Newton-Raphson Method

Newton's method is faster but evaluates the function $f(Y_{gw1})$ and its derivative.

The root estimate is provided by,

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$

Newton's formula uses the 1st order derivative which is computed numerically:

$$f'(Y) \approx \frac{f(Y + dY) - f(Y)}{dY}$$

Solution can go out of the brackets especially near a horizontal asymptote.

Newton and Dichotomy method [4]

This method takes a bisection whenever Newton iterations would take the solution out of bounds of whenever the size of brackets is not reducing rapidly enough.

Brent method

On each iteration Brent's method approximates the function using an interpolating curve. On the first iteration this is a linear interpolation of the two endpoints. For subsequent iterations the algorithm uses an inverse quadratic fit to the last three points, for higher accuracy. The intercept of the interpolating curve with the x-axis is taken as a guess for the root. If it lies within the bounds of the current interval then the interpolating point is accepted, and used to generate a smaller interval. If the interpolating point is not accepted then the algorithm falls back to an ordinary bisection step. The best estimate of the root is taken from the most recent interpolation or bisection.

$$x = x_2 + \frac{P}{Q}$$

Where,

$$P = S\left[T(R - T)(x_3 - x_2) - (1 - R)(x_2 - x_1)\right]$$

$Q = (T-1)(R-1)(S-1)$ and $R \equiv \frac{f(x_2)}{f(x_3)}, S \equiv \frac{f(x_2)}{f(x_1)}, T \equiv \frac{f(x_1)}{f(x_3)}$.

The following table summarizes the each method's performance for one simple call,

	Dichotomy	Secant	Chord	Ridders	Newton	Newton& Dichotomy	Brent
Iterations	7	3	3	6	3	5	5
Run time (sec)*	0.004	0.003	0.003	0.002	0.003	0.002	0.002
Accuracy	1.d-06	1.d-06	1.d-06	1.d-08	1.d06	1.d-06	1.d-6
Solution	Yes	No	No	Yes	No	Yes	Yes

For 1,000,000 calls

	Dichotomy	Secant	Chord	Ridders	Newton	Newton& Dichotomy	Brent
Iterations	7	3	3	6	3	5	5
Run time*	1m58.6s	0m8.470s	0.8470s	1m33.833s	0m18.004s	3m17.780s	1m13.001s
Accuracy	1.d-06	1.d-06	1.d-06	1.d-08	1.d06	1.d-06	1.d-6
Solution	Yes	No	No	Yes	No	Yes	Yes

*Time estimation for an Intel (R) Celeron (R) CPU B815 @ 1.60GHz processor.

The reason that Secant (False Position), Chord and Newton-Raphson methods give different solution from the other methods and fail to give a solution that confirms initial equations for a temperature far away from T_{min}, is the way temperature criterion is determined: root search stops is the difference $T^{new} - T^{old}$ is smaller than the desired accuracy. This is why Ridders' method that uses different accuracy levels successes.

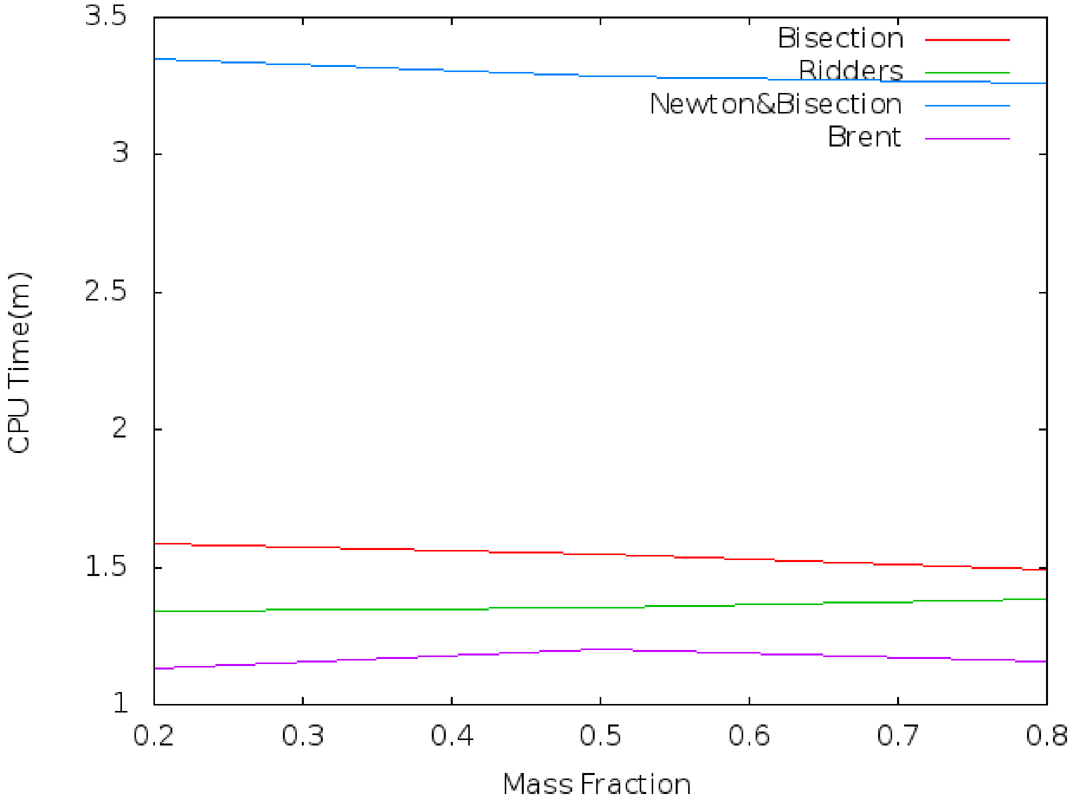


Figure 3. CPU time for 10^6 calls for different mass fractions.

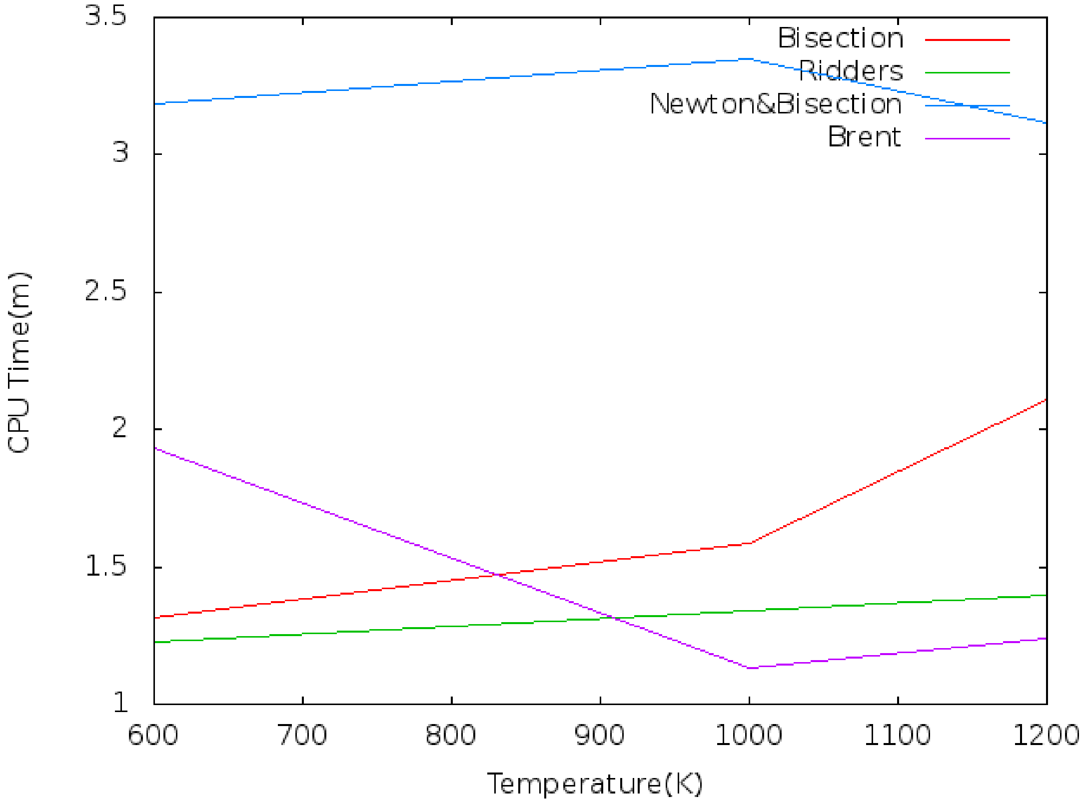


Figure 4. CPU time for 10^6 calls for different temperatures.

3.4 Coupling with the Two-Phase model

To illustrate the method we coupled it with a two phase model [5]. The model allows two phases for multicomponent fluids and performs a relaxation of pressure. At the test case that follows there is a shock tube where in the first domain there is air with volume fraction 0.9 that contains air and vapor water (mass fraction is equal to 0.2) and pure water with volume fraction 0.10. The left part of the computational domain (high-pressure area) has pressure equal to 100bar and the right domain has 1bar (low-pressure area). Both domains have temperatures equal to 300K.

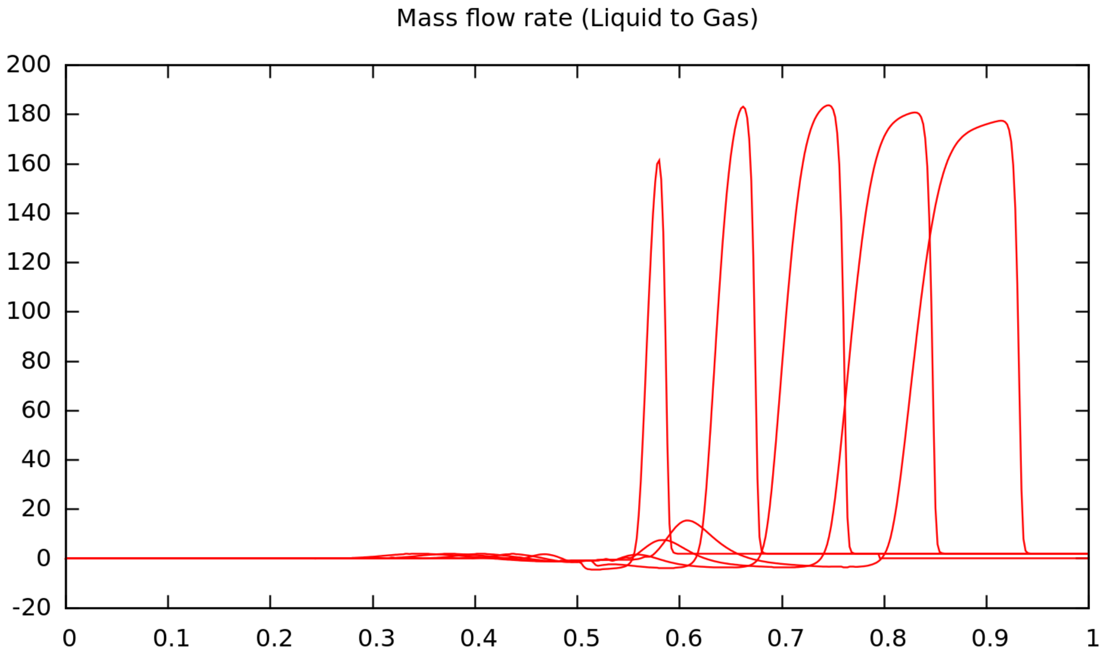


Figure 5. Mass flow rate in the shock tube through time evolution. In the shock wave region the amount of liquid that evaporates increases.

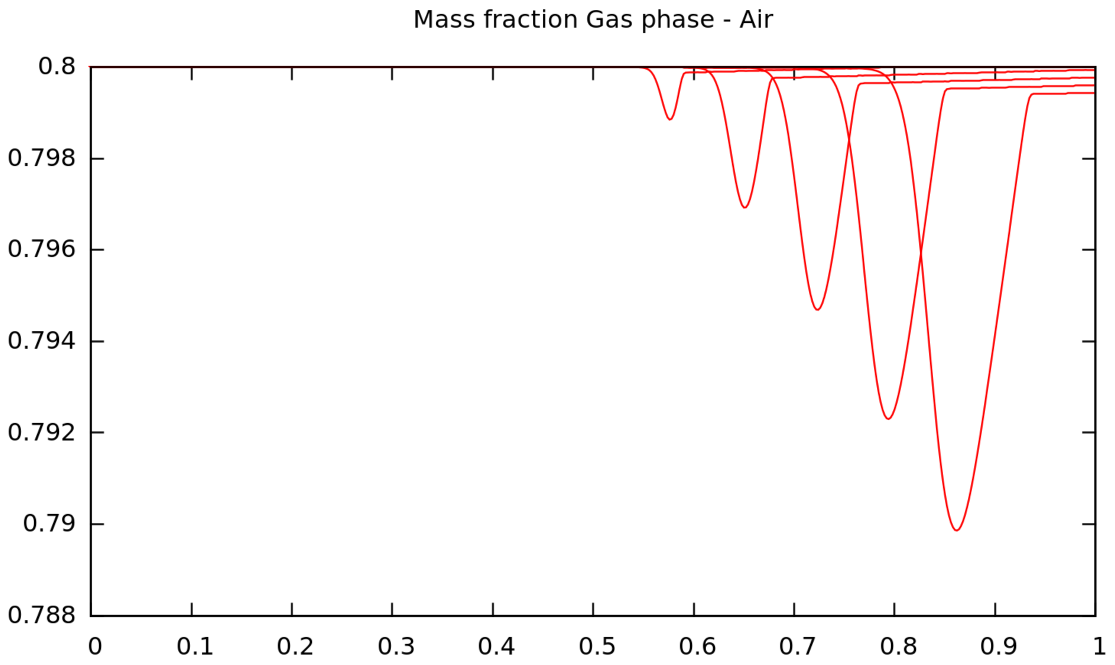


Figure 6**.** Mass fraction of gas phase in the shock tube through time evolution. It increases at the shock wave area.

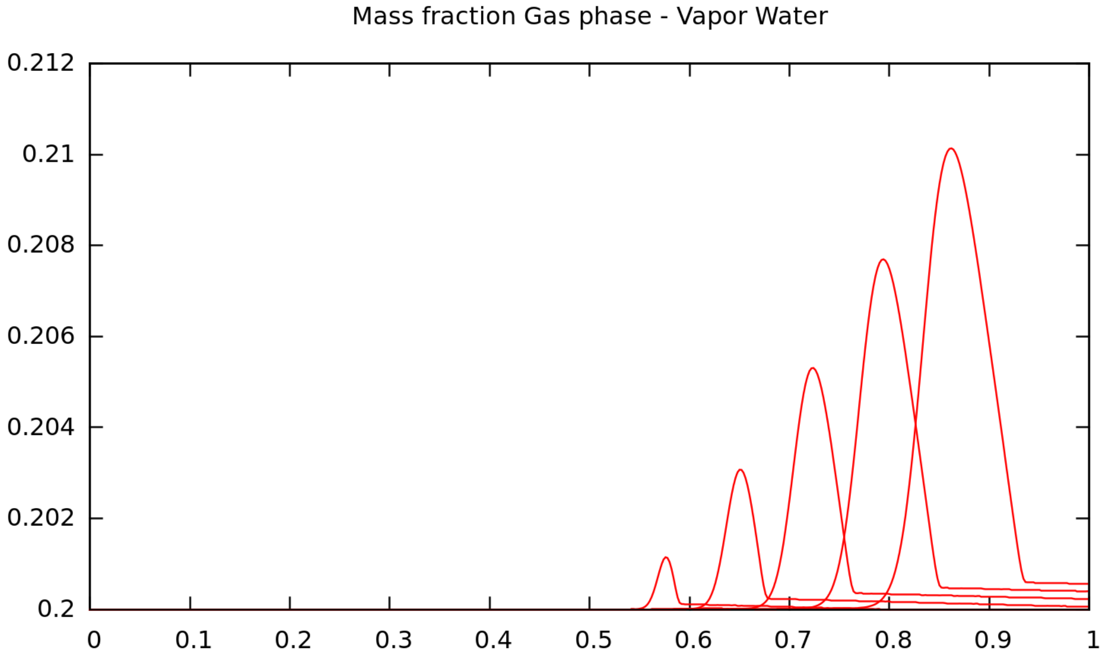


Figure 7. Mass fraction of liquid phase in the shock tube through time evolution. It decreases at the shock wave area.

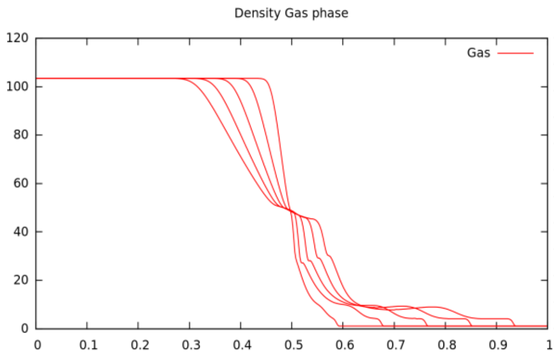


Figure 8a) Density of gas phase in the shock tube through time evolution.

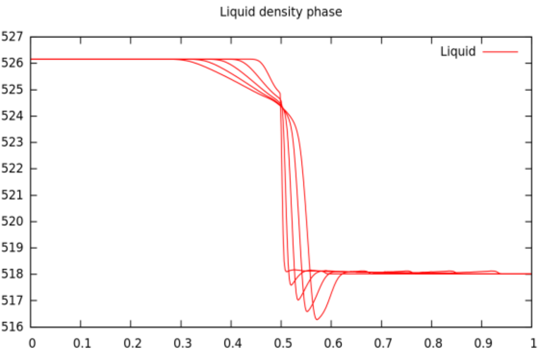


Figure 8b) Density of liquid phase in the shock tube through time evolution.

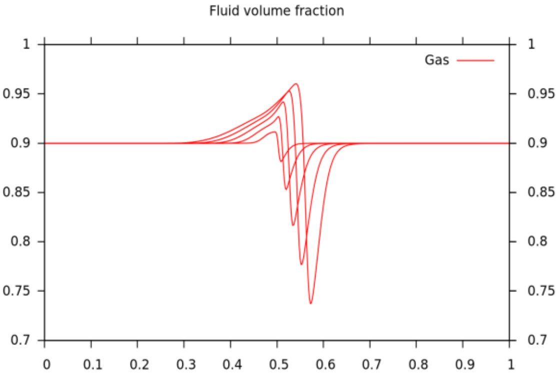


Figure 9a) Volume fraction of gas phase in the shock tube through time evolution.

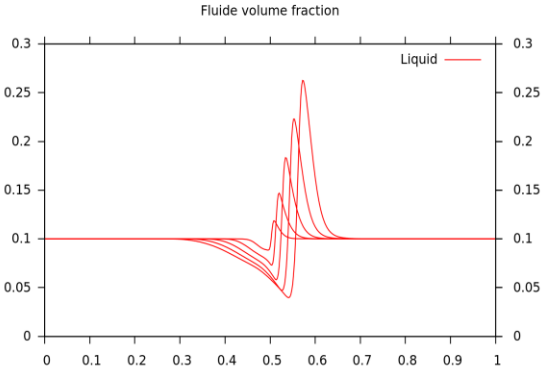


Figure 9a) Volume fraction of gas phase in the shock tube through time evolution.

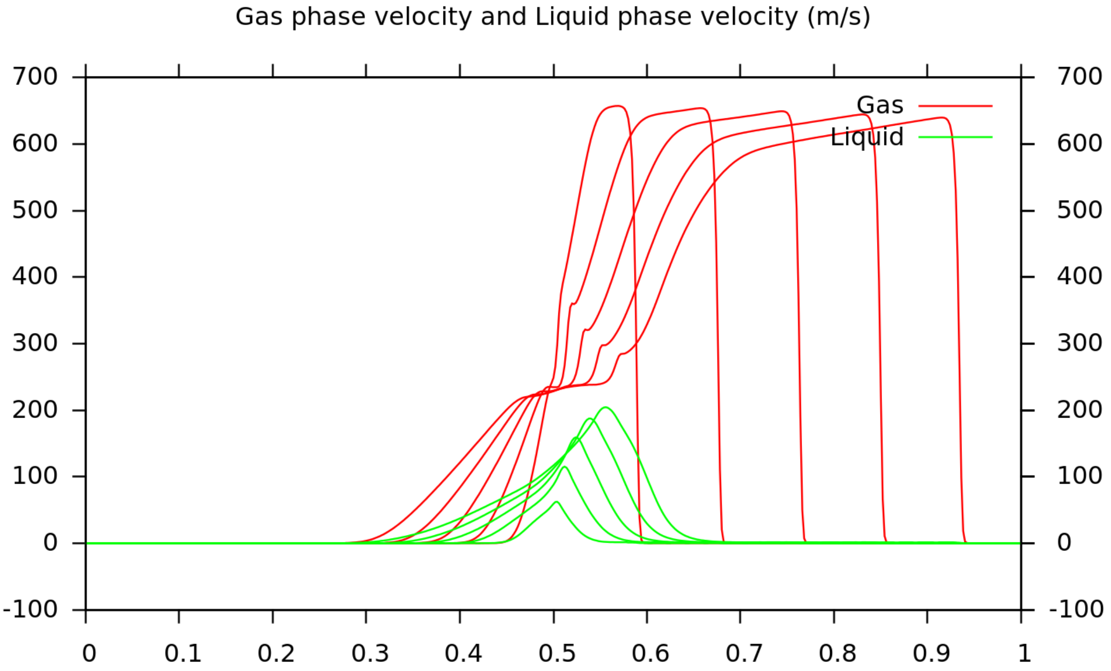


Figure 10. Velocities of both gas and liquid phases inside the tube, through time evolution.

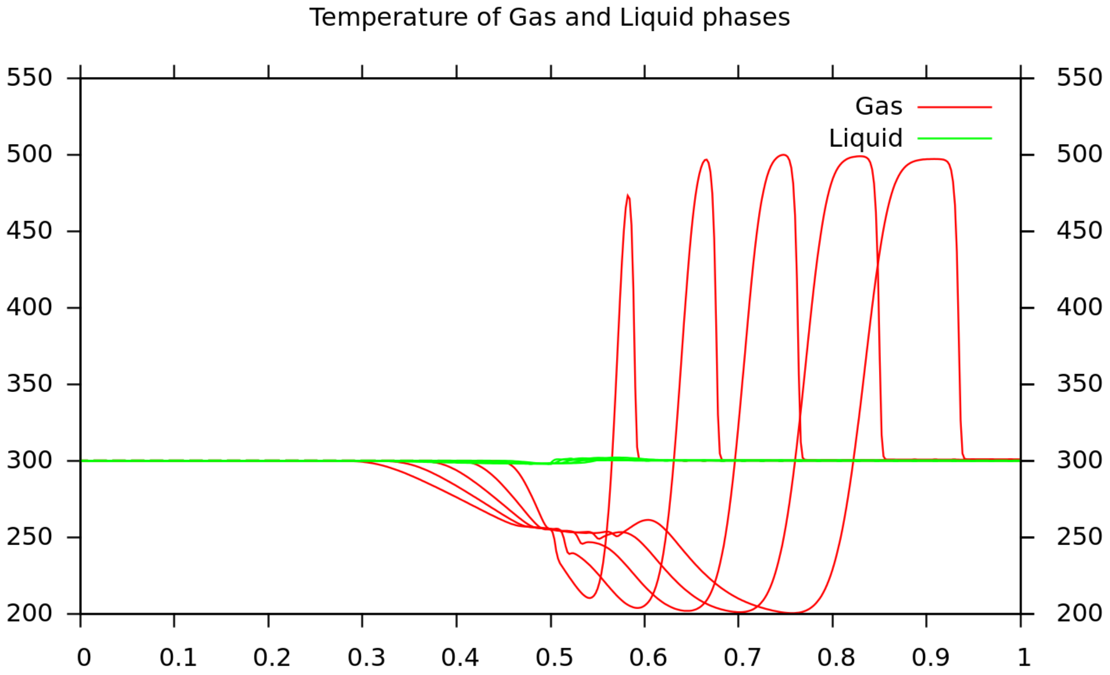


Figure 11. Temperatures of both gas and liquid phases inside the tube, through time evolution.

Initially we assume thermodynamic equilibrium and the vapor pressure is equal to its saturated value. The shock increases vapor pressure that leads to condensation. The drag force at the drops inside the gas phase causes a heat transfer from the gas to the drops. The latent heat that is released increases the temperature inside the drops. When the vapor pressure becomes smaller than the saturated vapor pressure, the drops start to evaporate causing the radius of the drops to change (fig. 12). In this case the heat transfer occurs from the drops to the gas. The rate that temperature changes, decreases. If the temperature in the high and low domain are initially the same, there will not be a uniform temperature between the shock wave and the expansion wave.

The mass flow rate is greater than zero and smaller at the high pressure domain where the expansion wave travels, but increases significantly in the area of the shock wave in the low pressure region. The expansion wave that travels in the left domain changes weaker the phase velocity, density and pressure whereas the shock wave more effectively them as expected. The reason that these changes do not occur with the same rate in the two phases is due to the difference in the compressibility of the fluids. Moreover at the left domain, water is forced to increase the pressure and decreases its volume fraction leading to an increase at air’s volume fraction (fig. 9a-9b). The exact opposite effects hold on the left domain.

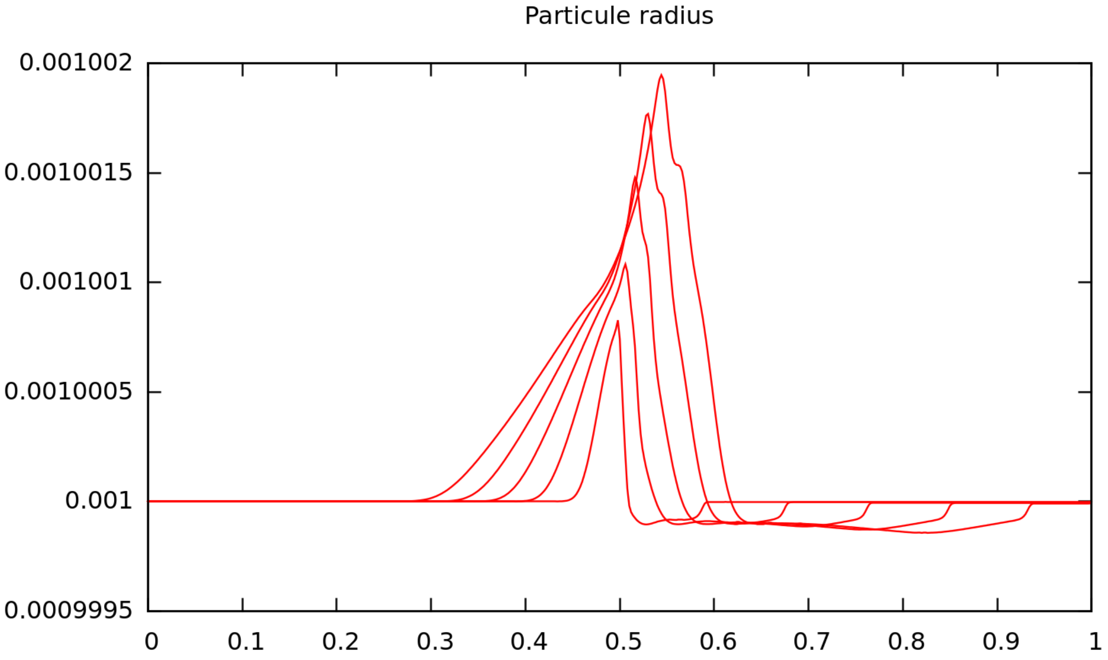


Figure 12. Radius of a single drop in the shock tube through time evolution for uniform temperature at 300K.

Appendix A – Chemical equilibrium

Each chemical reaction involves reactants and products. In chemical equilibrium the concentrations on both sides of the reaction are time invariant.

Introducing the chemical potential μ as the partial molar free energy of a chemical species of a mixture with n species each one having N_i moles we have:

$$dG = -SdT + Vdp + \sum_{i=1}^{n} \mu_i dN_i$$

At thermal and mechanical equilibrium it reduces to:

$$dG = \sum_{i=1}^{n} \mu_i dN_i$$

Then each of the μ_i of species i can be explicitly defined as,

$$\mu_i = \left(\frac{\partial G}{\partial N_i} \right)$$

At chemical equilibrium, the system Gibbs free energy reaches its minimum. It means,

$$dG = 0$$

Which by the above definition gives,

$$\sum_{i=1}^{n} \mu_i dN_i = 0$$

Considering a liquid vapor phase change situation,

$$\mu_l dN_l + \mu_g dN_g = 0$$

Mass conservation implies,

$$dN_l + dN_g = 0 ,$$

as the liquid and gas molar masses are equal.

Therefore,

$$\left(\mu_l - \mu_g\right) dN_l = 0$$

As around equilibrium dN_l is small but non zero, the chemical equilibrium condition is now written as,

$$\mu_l = \mu_g$$

Appendix B – Equation of state

Stiffened Gas Equation of state (EOS)

The equation of state and the calculation of the conventional properties of the phase diagram and useful fluid quantities are described below. Stiffened gas which is applied (SG EOS) can be written as a pressure law:

$$p(\rho, e) = (\gamma - 1)\rho(\mathrm{e} - \mathrm{e}_*) - \gamma p_\infty$$

Where γ, e_* and p_∞ are parameters related to the fluid. Here e_* defines the zero point for the internal energy and becomes relevant when phase transitions are involved. The parameter p_∞ leads to the stiffed properties compared to ideal gases meaning that large values of p_∞ implies an almost incompressible behavior of fluid.

Calculation of flow properties:

$$\mathrm{e}(\mathrm{p}, \upsilon) = \frac{p + \gamma p_\infty}{\gamma - 1}\upsilon + q \qquad (1)$$

$$\upsilon(\mathrm{p}, \mathrm{T}) = \frac{(\gamma - 1)\,\mathrm{C}_\upsilon T}{p + \gamma p_\infty} \qquad (2)$$

$$h(T) = \gamma C_{\upsilon} T + q \tag{3}$$

$$g(p,T) = (\gamma C_{\upsilon} - q^{'})T - C_{\upsilon} T \log \frac{T^{\gamma}}{(p + p_{\infty})(\gamma - 1)} + q \tag{4}$$

where e is the specific internal energy, h is the enthalpy, p the pressure, $\upsilon = 1/\rho$ the specific volume, T is the temperature, g the Gibbs free energy and $\gamma, p_{\infty}, C_{\upsilon}, q, q^{'}$ are specific fluid constant.

A method to determine the above quantities in two phase systems is given in Le Metayer *et al. (2004)*. The coupling of gas and liquid parameters is particularly examined.

Computation method

The parameters involved in the SG EOS are determined from experimental curves for each fluid. In the case of liquid evaporation saturation curves are considered:

$$p = p_{sat}(T), h_{l,\exp}(T), h_{g,\exp}(T), \upsilon_{l,\exp}(T), \upsilon_{g,\exp}(T)$$

and the latent heat of evaporation $L_{v,\exp}(T) = h_{g,\exp}(T) - h_{l,\exp}(T)$

- From equation of enthalpy (c) we have:

$$\frac{dh_k}{dT} = \gamma_k C_{\upsilon,k} = C_{p,k} \quad \text{for each k=l,g}$$

Heat capacity factors $C_{p,k}$ can be determined by a linear interpolation between two reference states 0 and 1 as:

$$C_{p,k} = \frac{h_{k,\exp}(T_1) - h_{k,\exp}(T_0)}{T_1 - T_0} \qquad \text{for each k=l,g}$$

Reference energies are now expressed as:

$$q_k = h_{k,\exp}(T_0) - C_{p,k} T_0 \qquad \text{for each k=l,g}$$

- With the saturation pressure curve $p = p_{sat}(T)$ the specific volume is:

$$\upsilon_k(T) = \frac{(C_{p,k} - C_{\upsilon,k})T}{(p_{sat}(T) + p_{\infty,k})} \quad \text{for each k=l,g} \tag{5}$$

The relation may be written with logarithms as:

$$d\log(\upsilon_k(T)) = d\log(T) - d\log(p_{sat}(T) + p_{\infty,k}) \quad , \text{ for each k =l,g}$$

Integration between the two reference states 0 and 1 yields:

$$\log(\upsilon_{\mathrm{k}}(T_1)) - \log(\upsilon_{\mathrm{k}}(T_0)) = \log(\mathrm{T}_1) - \ln(\mathrm{T}_0) - \log(p_{sat}(T_1) + \mathrm{p}_{\infty,k}) + \log(p_{sat}(T_0) + \mathrm{p}_{\infty,k})$$

Solving for $\mathrm{p}_{\infty,k}$ we get:

$$\mathrm{p}_{\infty,k} = \frac{\upsilon_{\mathrm{k}}(T_0)T_1 p_{sat}(\mathrm{T}_0) - \upsilon_{\mathrm{k}}(T_1)T_0 p_{sat}(\mathrm{T}_1)}{\upsilon_{\mathrm{k}}(T_1)T_0 - \upsilon_{\mathrm{k}}(T_0)T_1} \qquad \forall k = l, g$$

- Equation (5) applied to the reference state 0 provides the approximation of the heat capacity factor $\mathrm{C}_{\upsilon,k}$:

$$\mathrm{C}_{\upsilon,k} = \mathrm{C}_{\mathrm{p},k} - \frac{\upsilon_k(\mathrm{T}_0)}{T_0(p_{sat}(T_0) + p_{\infty,k})} \qquad \forall k = l, g$$

- Constant γ_k now is:

$$\gamma_k = \frac{\mathrm{C}_{\mathrm{p},k}}{\mathrm{C}_{\upsilon,k}} \qquad \forall k = l, g$$

- At thermodynamic equilibrium the two Gibbs free energies have to be equal $g_g = g_l$. This implies:

$$\log(p + p_{\infty,\upsilon}) = A + \frac{B}{T} + C\log(T) + D\log(p + p_{\infty,1}) \qquad (6)$$

Where constants A, B, C and D that depend on the SG EOS parameters with the following correlations:

$$A = \frac{C_{p,l} - C_{p,\mathrm{g}} + q'_g - q'_l}{C_{p,\mathrm{g}} - C_{\upsilon,\mathrm{g}}}, \mathrm{B} = \frac{q_l - q_g}{C_{p,\mathrm{g}} - C_{\upsilon,\mathrm{g}}}, \mathrm{C} = \frac{C_{p,\mathrm{g}} - C_{\mathrm{p,l}}}{C_{p,\mathrm{g}} - C_{\upsilon,\mathrm{g}}} \text{ and}$$

$$D = \frac{C_{p,1} - C_{\upsilon,1}}{C_{p,\mathrm{g}} - C_{\upsilon,\mathrm{g}}}.$$

Relationship (6) is non-linear but permits the computation of the theoretical curve $p = p_{sat}(T)$. Entropy constants (q') are also needed for each phase. To do this we consider that $q'_l = 0$ and choose a q'_g to fit properly with the experiments curves.

Mixture SG EOS

For a mixture containing 2 species with mass and volume fractions $Y_1, Y_2, \alpha_1, \alpha_2$ respectively the internal energy is defined as:

$$\rho e = \alpha_1 \rho_1 e_1 + \alpha_2 \rho_2 e_2$$

By using the SG EOS (1) each product $\rho_k e_k$ can be written as:

$$\rho_k e_k = \frac{p_k + \gamma_k p_{\infty,k}}{\gamma_k - 1} + \rho_k q_k$$

The pressure of the mixture is now expressed with:

$$p(\rho, e, \alpha_1, \alpha_2, \mathrm{Y}_1, \mathrm{Y}_2) = \frac{\rho(e - \mathrm{Y}_1 q_1 - \mathrm{Y}_2 q_2) - (\frac{\alpha_1 \gamma_1 p_{\infty,1}}{\gamma_1 - 1} + \frac{\alpha_2 \gamma_2 p_{\infty,2}}{\gamma_2 - 1})}{\frac{\alpha_1}{\gamma_1 - 1} + \frac{\alpha_2}{\gamma_2 - 1}}$$

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