Surface Condensation and Evaporation in Turbulent Flows

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Abstract:

In the context of the development of a bio-decontamination system, numerical modelling is required to ensure that condensation occurs on all of the volume to purify. Because this system must be adapted for various conditions and scales, the developed CFD model must accurately predict the physical mechanisms governing this type of flow. In the context of the ECOBIOCLEAN project, the adaptation of a CFD code with the implementation of the main mechanisms is explained, identified as condensation and evaporation, multicomponent diffusion, chemical decomposition, heat transfer and turbulence. The validation of the code is conducted in accordance to the literature and a comparison with the experimental results gathered with a prototype available at the Faculty of Pharmacy of Strasbourg is performed.

Mots clefs : CFD, évaporation, condensation, diffusion.

1 Introduction

A bio-decontamination system is being developed and a prototype has been built to test the conditions required to purify a volume. Since this system will be adapted for various applications of different scales, the model has to be able to correctly model the system for any geometry and dimensions, from a small test volume to a full scale clean room. Computational Fluid Dynamics, or CFD, is the most adaptable and accurate way to predict the behavior of the fluids.
The system consists in a heater and an injector in a circuit which can be closed or opened.

During the first phase, the decontamination phase, a solution of hydrogen peroxide is sprayed in a hot air stream. The droplets evaporate quickly, before reaching the volume to be decontaminated. There, condensation begins to form on the cold walls. The circuit is closed in order to conserve the hydrogen peroxide, to minimize the amount of solution to be consummed.

When all of the walls are covered with condensed hydrogen peroxide, the second phase begins, during which hot and dry air is blown in the volume. The circuit is now opened, letting out the vapor not needed anymore. This lasts until all of the hydrogen peroxide has evaporated.

2 CFD Model

2.1 Presentation of the solver

The CFD code used in the present work is called NSIBM, standing for Navier-Stokes Immersed Boundary Method. It is an massively paralllel incompressible Navier-Stokes solver developed at the ICube Laboratory, Strasbourg, France. It uses unstructured cartesian meshes, where the boundaries that cannot be modelled using only the cartesian mesh are modelled using the Immersed Boundary Method with an automatic mesh refinement along the boundary. The implemented schemes include the 1st and 2nd order for time and 1st to 3rd (TVD) for space. Turbulence can be modeled by Spalart-Allmaras, $k-\epsilon$ and $k-\omega$ models.

The code has been validated using standard cases from the literature, such as the driven cavity [1] and the buoyancy driven cavity [9] cases.

2.2 Model implementation

Modelling the decontamination system requires the implementation of several models, amongst which are the condensation and evaporation rate, multicomponent transport diffusion, chemical decomposition and the heat transfer.

- Vapor transport and diffusion: initially, there is no vapor in the volume. It is injected at the inlet. The driving parameter is the total mass of solution sprayed in the volume. It is sprayed at a certain rate until the saturation is reached.
- Condensation and evaporation happen on the walls. It can be expressed as a boundary condition. Different laws have been suggested by many authors to model the condensation or evaporation rate. The driving parameters are the vapor pressure and the temperature of the vapor close to the wall, and the saturation vapor pressure at the boundary which is expressed as a function of the condensation temperature.
- Heat transfer. Modelling condensation requires an accurate modelling of the temperature difference between the liquid, on the wall, and the vapor. This requires an accurate modelling of the heat transfer of the condensation to the wall (and the outside) and to the gas stream.
- Chemical decomposition. One of the main advantages of using hydrogen peroxide for decontamination is its decomposition into water and oxygen, two friendly chemical components to the atmosphere and the human. With increasing temperature, the reaction rate will increase. This is not wanted during the first phase, since decontamination requires the hydrogen peroxide, but is during the second phase (rinse cycle).
### 2.2.1 Vapor transport

The assumption of quickly evaporating droplets leading to a single-phase flow, the problem only of mass transfer revolves around the diffusion of the condensables in the flow.

Each component $k$ is represented by its volume fraction $\alpha_k$, its molar fraction $x_k$ or its mass fraction $\omega_k$ in the flow. The perfect gas assumption leads to having the following equality: $\alpha_k = x_k$.

The general multiphase Navier-Stokes mass balance equation for incompressible flows writes:

$$\frac{\partial \alpha_k}{\partial t} + \nabla \cdot (\alpha_k \mathbf{V}_k) = -\frac{1}{\rho_k} \nabla \cdot \mathbf{J}_k + \frac{\Gamma_k}{\rho_k}$$

where $\mathbf{J}_k$ is the diffusion flux of the vapor in the mixture. This flux can be divided into several diffusion fluxes, each accounting for a diffusion cause, molecular diffusion, turbulence induced diffusion and thermal diffusion:

$$\mathbf{J}_{k,\text{mass}} = \mathbf{J}_{k,\text{mol}} + \mathbf{J}_{k,\text{turb}} + \mathbf{J}_{k,\text{th}}$$

In binary mixtures, the molecular diffusion flux in terms of mass fraction gradient are commonly defined as:

$$\mathbf{J}_{\text{i, mol}} = -\rho \mathbf{D}_{i,j} \nabla \omega_i$$

$$= -\rho D_{i,j} \frac{M_i M_j}{M^2} \nabla x_i$$

For the multi-component mixtures, the model uses a mixture-averaged diffusion coefficient, based on calculations from Kee et al. [3] and Sutton and Gnoffo [7]:

Using mass fraction

$$\mathbf{J}_{\text{i, mol}} = -\rho \mathbf{D}_{i}^{\text{Mix}} \nabla \omega_i$$

or, using mole fraction,

$$\mathbf{J}_{\text{i, mol}} = -\rho \mathbf{D}_{i}^{\text{Mix}} \frac{M_i}{M} \frac{1 - \omega_i}{1 - x_i} \nabla x_i$$

with

$$D_{i}^{\text{Mix}} = \frac{\sum_{j \neq i} x_j M_j}{\sum_{j \neq i} x_j / D_{ji}}$$

The turbulence adds an effect of diffusion. It is often caracterised by a turbulent Schmidt number. Similarly to molecular diffusion, the turbulent Schmidt number is defined as:

$$Sc_t = \frac{\mu_t}{\rho D_t}$$

where $\mu_t$ is the eddy viscosity. This leads to the expression of the turbulent diffusion coefficient, which is directly used to model the turbulent diffusion:
\[ \overrightarrow{J_{i,\text{turb}}} = -\rho D_i \nabla \omega_i \] (9)

\[ D_i = \frac{\mu_i}{\rho Sc_i} \] (10)

Tominaga and Stathopoulos [8] reviewed the studies regarding the turbulent Schmidt number used in the literature. Mainly, the values of the turbulent Schmidt number used are 0.7 or 0.9. However, in a significant number of cases, experimental values can go from 0.2 to 1.3, depending on flow parameters and the geometry.

2.2.2 Condensation and evaporation models

It is the main mode of condensation of this study. This mode happens because the hot gas stream encounters the cold wall to which transfers heat and thus, cools down. The condensables phase then changes on the walls, at a rate depending on several parameters.

Herz-Knudsen-Schrage equation: Marek and Straub [5] suggest using the Herz-Knudsen-Schrage equation, defined as :

\[ \dot{m}_v = \frac{2}{2 - K_C} \cdot \left( \frac{M}{2\pi R} \right)^{1/2} \cdot \left[ K_C \cdot \frac{p_v}{T_v^{1/2}} - K_E \cdot \frac{p_{\text{sat}}(T_l)}{T_l^{1/2}} \right] \] (11)

where \( K_C \) and \( K_E \) are respectively the condensation and the evaporation coefficients. They are defined as follows :

\[ K_C = \frac{\text{number of gaseous molecules absorbed by the liquid phase}}{\text{number of gaseous molecules impinging the liquid phase}} \] (12)

\[ K_E = \frac{\text{number of liquid molecules absorbed by the gaseous phase}}{\text{number of liquid molecules emitted by the liquid phase}} \] (13)

This equation has been used in many studies and is not subject to approximation as it does not need data about the heat transfer coefficient, contrary to the following correlations. It also has the advantage of being a reversible equation, meaning that this can be used to account for condensation and evaporation.

Heat and Mass Transfer Analogy: Another way of estimating the condensation is suggested by Liu et al. [4] who studied the condensation in a building. They used the Lewis equation, and assumed a constant heat transfer at the boundaries, directly linking the heat transfer rate to the mass transfer rate. It will be referred to as the Heat and Mass Transfer Analogy (HMTA) :

\[ \dot{m}_v = \frac{hT}{c_p} L_e^{-2/3} \left( x_v - \frac{p_{\text{sat}}(T_l)}{p} \frac{T_v}{T_l} \right) \] (14)

where \( L_e = \frac{Sc}{Pr} = \frac{\alpha}{D} \) (15)
Both condensation models will be studied and compared to the results obtained with the prototype of the bio-decontamination system.

### 2.2.3 Wall heat transfer

According to all of the studies regarding condensation, the temperature difference between the bulk gas and the liquid phase is a leading parameter in condensation. Therefore, an accurate modelling of heat transfer is crucial to the study of condensation.

The temperature distribution in the bulk flow is calculated accurately with the classical convection-diffusion equation.

If the condensation is represented by a continuous film on the walls, the heat transfer model is simplified. In this case, the condensation can be represented by an extra resistance between the bulk flow and the outside. The following thermal/electrical anology can be made to analyze the temperature profile. It is assumed that there is no convection resistance between the liquid film and the wall. Also, due to the phase change, an amount of heat corresponding to the latent heat of vaporization is released during condensation. Herrantz et al. [2] suggests adding this mechanism in parallel to the convection.

![Thermal/electrical analogy of the wall heat transfer for filmwise condensation.](image)

The heat flux can thus be expressed as follows:

\[
q = h_{\text{f}}(T_g - T_{\text{ext}}) = \frac{T_g - T_{\text{ext}}}{\frac{R_{1f}R_{\text{cond}}}{R_{1f} + R_{\text{cond}}} + R_{2f} + R_3 + R_4}
\]  

(16)

**Condensation heat transfer**

Condensation generates energy, which was stored in the gas as latent heat of vaporization. This heat is released during condensation.

\[
q_{\text{cond}} = h_{\text{cond}}(T_g - T_i) = \dot{m}L_v
\]  

(17)
Using the Sherwood number formulation, the heat transfer coefficient expression is

\[
h_{\text{cond}} = \frac{1}{R_{\text{cond}}} = \frac{Sh}{L} \frac{M_v L_v D}{R} \left( \frac{P_v - P_{\text{sat}}}{T_g - T_i} \right)
\]  

(18)

Herrantz et al. [2], based on the work of Peterson et al. [6] relative to the diffusion layer theory, suggest making the approximation (19), using the Clapeyron equation (20) and making another approximation for the specific volume change (21).

\[
\frac{P_v}{T_g} - \frac{P_{\text{sat}}}{T_i} \approx \frac{1}{T_{\text{avg}}} (P_v - P_{\text{sat}})
\]  

(19)

\[
\frac{\Delta P}{\Delta T} = \frac{L_v}{T_{vfg}}
\]  

(20)

\[
v_{fg} = v_g - v_l = \frac{R T_i}{P_v M_v} - v_l \approx \frac{R T_i}{P_v M_v}
\]  

(21)

After developing, the following expression is obtained:

\[
h_{\text{cond}} = \frac{Sh}{L} \frac{P_v M_v^2 L_v^2 D}{R^2 T_g T_i} \Phi
\]  

(22)

where \( \Phi \) is the ratio between the log mean molar fractions of vapor and noncondensables in the boundary layer. This factor is added to correct the result with empirical observations on the effect of condensable concentration.

\[
\Phi = \frac{x_{v,\text{avg}}}{x_{\text{nc,avg}}} = -\ln \left[ \frac{1 - x_{\text{nc,b}}}{1 - x_{\text{nc,i}}} \right] \frac{\ln \left[ \frac{x_{\text{nc,b}}}{x_{\text{nc,i}}} \right]}{\ln \left[ \frac{x_{v,\text{avg}}}{x_{\text{nc,avg}}} \right]}
\]  

(23)

**Convection between the wall and the exterior**

The wall is passively cooled down with ambient temperature due to free convection with the exterior. The McAdams correlation, valid for Rayleigh numbers in the range of \( 10^9 < Ra < 10^{12} \) and independent of the characteristic length, is used:

\[
Nu = 0.13 Gr^{1/3} Pr^{1/3}
\]  

(24)

\[
\Rightarrow h_4 = \frac{1}{R_4} = 0.13 \left[ \frac{g \rho_{\text{ext}} C_{p,\text{ext}}^2 \lambda_{\text{ext}}^2 |T_w - T_{\text{ext}}|}{\nu_{\text{ext}} T_{\text{ext}}} \right]^{1/3}
\]  

(25)
## Nomenclature

### Constants and Variables

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>D</td>
<td>Diffusion coefficient</td>
<td>$m^2.s^{-1}$</td>
</tr>
<tr>
<td>$\bar{D}$</td>
<td>Binary diffusion coefficient</td>
<td>$m^2.s^{-1}$</td>
</tr>
<tr>
<td>$h$</td>
<td>Heat transfer coefficient</td>
<td>$W.K^{-1}.m^{-2}$</td>
</tr>
<tr>
<td>$J$</td>
<td>Diffusion flux</td>
<td></td>
</tr>
<tr>
<td>$L$</td>
<td>Characteristic length</td>
<td>$m$</td>
</tr>
<tr>
<td>$L_v$</td>
<td>Latent heat of vaporization</td>
<td>$J.kg^{-1}$</td>
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<tr>
<td>$M$</td>
<td>Molar mass</td>
<td>$kg.mol^{-1}$</td>
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<tr>
<td>$\dot{m}$</td>
<td>Condensation mass flux</td>
<td>$kg.s^{-1}.m^{-2}$</td>
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<tr>
<td>$P, p$</td>
<td>Pressure, partial pressure</td>
<td>$Pa$</td>
</tr>
<tr>
<td>$q$</td>
<td>Heat flux per unit surface</td>
<td>$W.m^{-2}$</td>
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<tr>
<td>$R$</td>
<td>Thermal resistance</td>
<td>$(W.K^{-1}.m^{-2})^{-1}$</td>
</tr>
<tr>
<td>$R$</td>
<td>Universal gas constant</td>
<td>$J.K^{-1}.mol^{-1}$</td>
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<tr>
<td>$\nu$</td>
<td>Specific volume</td>
<td>$m^3.kg^{-1}$</td>
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<tr>
<td>$V$</td>
<td>Velocity</td>
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<tr>
<td>$x$</td>
<td>Mole fraction</td>
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<td>$\lambda$</td>
<td>Thermal conductivity</td>
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<tr>
<td>$\rho$</td>
<td>Density</td>
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<tr>
<td>$\omega$</td>
<td>Mass fraction</td>
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### Subscripts and Superscripts

<table>
<thead>
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<tr>
<td>avg</td>
<td>Average</td>
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<tr>
<td>b</td>
<td>Bulk</td>
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<tr>
<td>ext</td>
<td>Exterior, outside</td>
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<tr>
<td>f</td>
<td>Film</td>
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<tr>
<td>g</td>
<td>Gas</td>
</tr>
<tr>
<td>$i, j, k$</td>
<td>Variable integer subscript</td>
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<tr>
<td>l</td>
<td>Liquid</td>
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<tr>
<td>m</td>
<td>Mass</td>
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<tr>
<td>nc</td>
<td>Non-condensable gas</td>
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<tr>
<td>sat</td>
<td>Saturation</td>
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<td>t</td>
<td>Turbulence</td>
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<tr>
<td>T</td>
<td>Thermal</td>
</tr>
<tr>
<td>v</td>
<td>Vapor, condensable</td>
</tr>
<tr>
<td>w</td>
<td>Wall</td>
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### Dimensionless numbers

<table>
<thead>
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<tr>
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<tr>
<td>$Pr$</td>
<td>Prandtl number</td>
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<tr>
<td>$Re$</td>
<td>Reynolds number</td>
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<tr>
<td>$Sc$</td>
<td>Schmidt number</td>
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## Références

1982.


