Use of Computational Fluid Dynamics in the Analysis of a Portable Wind Tunnel for Sampling of Odorous Emissions at Liquid Surfaces

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Enclosure sampling devices, such as wind tunnels and flux chambers, are commonly applied to quantify the emission rate of odorous compounds at passive liquid surfaces. As the aerodynamics of such devices is of great importance for the accuracy of results, proper evaluation methods are highly desired. Computational Fluid Dynamics (CFD) is one of these potential tools, to be used in complement to other methodologies. This paper is aimed to discuss aspects related to the use of CFD in the analysis of a wind tunnel device for sampling of odorous emissions at liquid surfaces. A CFD simulation of the wind tunnel that was developed at the University of New South Wales (UNSW wind tunnel) is used as an example-case to develop the discussion, describing the general steps that comprise a CFD study. Special attention is given to the validation step, exploring and discussing possibilities of validation against experimental data and theoretical models. It is shown, for this case, validation using published experimental data is particularly difficult. On the other hand, comparison with a theoretical boundary layer model suggests that the simulation represented an ideal (two-dimensional) situation for the wind tunnel, presenting an expected slightly difference in comparison with Blasius boundary layer description. Such deviations as well as the potential effect of a three-dimensional geometry are important considerations when dealing with practical situations.

1. Introduction

The emission rate of odorous compounds at passive liquid surfaces can be directly quantified by using sampling devices (such as flux chambers, hoods and wind tunnels), which are able to enclosure minimal parts of the emitting surface, so that the emitted compounds are captured by an air flow passing through the sampling system (Hudson and Ayoko, 2008; Capelli et al., 2013). Although broadly adopted (at much extend, due to its simplicity and low cost (Hudson and Ayoko, 2008; Capelli et al., 2013)), the use of flux hood method is subjected to two important concerns regarding to the aerodynamics of the sampling devices (Hudson and Ayoko, 2008): (i) the possibility of compounds accumulating in the sampling headspaces and (ii) an eventual inability of reproducing relevant features of atmospheric air flow. In both of these cases, the emission process can be greatly affected, leading to inaccurate results (Hudson and Ayoko, 2008).

Computational Fluid Dynamics (CFD) (i.e., the computational numerical solution of transport equations that describe the conservation of properties inherent to flow, as momentum, energy and mass of chemical species) constitutes a tool with great potential to contribute for the analysis of enclosure devices, being able to address the above mentioned points as well as other aspects related to their aerodynamics, as

development of boundary layers, for example. However, few studies reported the used of this technique for such purposes.

Saha et al. (2011) simulated the turbulent air flow and ammonia transportation inside wind tunnels of different sizes. The emission source (in CFD simulations and in the validation experiments) was represented by a liquid surface located at the measurement section of the wind tunnels. A rectangular parallelepiped-shaped domain was considered, indicating the assumption that the influence of inlet and outlet sections geometry can be completely represented by the boundary conditions adopted for the flow in the measurement section, which was indeed coherent with the apparatus used in the experimental validation. Simulation results suggested that inlet velocity and wind tunnel size can present a relevant effect on momentum and concentration boundary layers close to the liquid surface, consequently influencing emissions.

Eckley et al. (2010) and Lin et al. (2012) applied CFD simulations and laboratory experiments to study and improve flow through equipment for direct measurement of mercury fluxes from soils. Despite these studies focused on devices designed for assessment of mercury emissions at solid/porous surfaces (soils), they are noteworthy for including some detailed geometrical features (e.g., entrance holes and outlet section, depending on the case) and also for exemplify additional ways to explore results.

This paper presents a discussion on the use of CFD technique as a tool to analyze a wind tunnel device for sampling of odorous emissions at liquid surfaces. The discussion is developed along with a exemplification case constituted by the simulation of air flow and transportation of chemical species in a two-dimensional representation of the wind tunnel that was developed at the University of New South Wales, Australia (UNSW wind tunnel) in the 1990's (Jiang et al., 1995) and which has been tested and improved since then (Wang et al., 2001).

2. Numerical simulation

2.1 Computational domain

A schematic drawing of the UNSW wind tunnel (displaying the original design from Jiang et al., 1995) is presented in Figure 1a. Inlet air is pumped by an external fan through a carbon filter followed by a flexible tube that connects to the extension inlet duct. An expansion section containing flat vanes and a baffle fitted between the expansion section and the main section are intended to improve uniformity of the inlet flow. The bottom of the whole main section (measurement section) is open and stays in contact with the liquid surface. The central longitudinal planes of the main section, the contraction section and the mixing chamber of the UNSW wind tunnel were chosen as computational domain, assuming a two-dimensional (2D) configuration (whose contour is identified in Figure 1a). The attempting to simulate a 2D geometry – which means to assume that side walls influence is reasonably restrict and negligible – is motivated by the mass transfer modelling and experimental investigation of Bliss et al. (1995), where a 2D description of the mass transfer boundary layer was considered.

2.2 Numerical model and boundary conditions

Air flow and ammonia dispersion inside the wind tunnel are governed by the conservation equations of mass, momentum and mass of chemical species (ammonia). Flow was assumed laminar, in accordance with qualitative indications about the flow, reported by Jiang et al. (1995) and Hudson (2009), and with mass transfer results of Bliss et al. (1995). Equations were solved for isothermal (15 °C), incompressible and steady state conditions, considering that the wind tunnel was supposed to be operating in such conditions in the experiments chosen for validation (Bliss et al., 1995). Concerning to steady state, Bliss et al. (1995) argue that variations (with time) on ammonia concentration at the liquid surface were so small that could be neglected. Isothermal condition was also adopted by Saha et al. (2011); although authors made no comments about the properness of this assumption, their relatively good validation results enforce its adoption in here. Air density (1.226 kg m^{-3}) and viscosity (1.797 × 10^{-5} kg m^{-1} s^{-1}) were calculated according to McQuillan et al. (1984). Ammonia diffusivity in air (2.017 × 10^{-5} m^{2} s^{-1}) was the same value adopted by Bliss et al. (1995).

Boundary conditions types are identified on Figure 1b. A uniform inlet velocity profile of 0.33 m s^{-1} was considered in order to match experiments of Jiang et al. (1995) and Bliss et al. (1995). Non-flux and non-slip conditions were imposed at wind tunnel walls. At the liquid surface, such conditions were also assumed, considering that the (quiescent) water surface behaves as a wall under low air velocities – the same assumption was adopted, for example, in Saha et al. (2011). A zero differential pressure was set at the outlet of the mixing chamber, which was open to the atmosphere in the experiments.
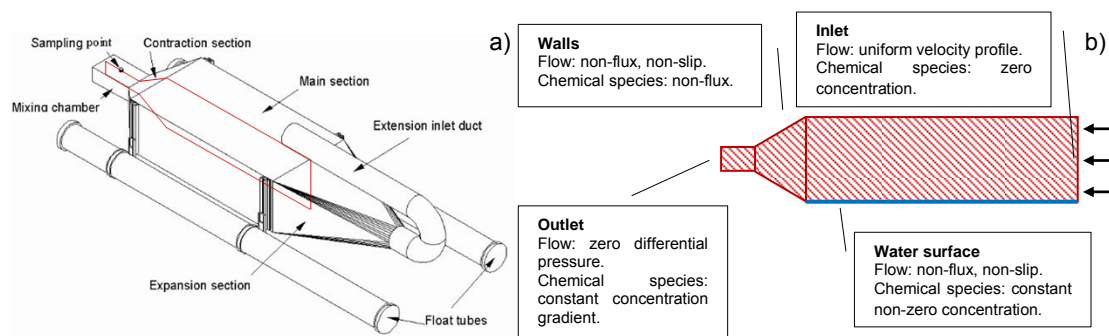
Figure 1: (a) schematic drawing *of UNSW wind tunnel (adapted from Jiang et al., 1995) identifying the contour of the computational domain and (b) boundary conditions types.*

For simulation of ammonia transportation, the inlet ammonia concentration was assumed to be zero (considering a "clean" inlet air). Ammonia zero-flux condition was set for wind tunnel walls and constant concentration gradient was considered at the mixing chamber outlet. A constant concentration of 2.680×10^{-4} kg m^{-3} was adopted at air-liquid interface; this value is coherent (applying Henry`s Law) with the expected ammonia concentration in the liquid solution used in the experiments of Bliss et al. (1995) – it has to be noted that such correspondence is not necessarily mandatory, once the boundary layer mass transfer coefficient is supposed to be dependant only on flow conditions (see Eq(1)).

2.3 Mesh and solution
A non-uniform structured grid was constructed, using the Ansys Package Meshing software, with hexahedral-shaped control volumes. Intense near-wall refinement was attempted once the main flow features and variations as well as mass transfer from the liquid surface are expected to take place in the near-wall boundary layer. Mesh sensitivity test comprised the evaluation of three grid sizes (32,925, 54,720 and 104,190 elements) considering two criteria: comparison of resulting vertical profiles for velocity and ammonia concentration at three different longitudinal positions, x = 0.2 m, x = 0.4 m and x = 0.6 m (representing 1/4, 1/2 and 3/4 of the main section length, respectively); and calculation of the Grid Convergence Index (GCI) (Roache, 1997), considering both the average wall shear and the vertical concentration gradient at the interface as solution functionals – these are important parameters in boundary layer chemical species transport. For solving the governing equations, Ansys CFX 13.0 software was chosen, running in parallel in a 4 core CPU (total 8 Gb RAM). Convergence criteria were: root mean squared (RMS) normalized residuals under 10^{-5}; and domain imbalance less than 1 % for mass, momentum and mass of ammonia fluxes.

3. Results and discussion

3.1 Mesh sensitivity test
Comparing the vertical profiles for velocity and ammonia concentration, it was verified that profiles present the same general shape for the three grid sizes, visually indicating good convergence. Relative differences between values at 200 equally spaced points in the profiles were indeed generally small. Following recommendations from Roache (1997), the finer grid (104,190 elements) was chosen, given that the results were already computed and no additional cases would be simulated. For this finer grid, GCI was 1.845 % and 1.407 %, for average wall shear and concentration gradient at interface, respectively.

3.2 Validation and further considerations
There is a range of potential errors that may mislead conclusions derived from simulation results, if these errors are not properly considered and treated when performing CFD simulations. Mesh sensitivity tests and observation of GCI, as reported above, are very important in order to verify if the solution is not significantly compromised by discretization errors (Roache, 1997). Additionally, one or more type of validation is strongly desirable to enhance confidence over the interpretation of results. The aim of

validation is to indicate if obtained results (or, in a broader sense, the whole modelling procedure) are reasonably able to represent a situation of practical importance in the problem being studied.

In the present case, vertical profiles at longitudinal positions x = 0.2 m, x = 0.4 m and x = 0.6 m resulting from CFD simulation were confronted to velocity values obtained through interpolation of experimental results reported by Jiang (1993) at five vertical positions inside the UNSW wind tunnel operating with air velocity of 0.33 m s^{-1}, as depicted in Figure 2a. A good agreement between simulation and experimental profiles is not observed. Possibly, the main reason for such apparent disparity is that the inlet boundary condition (uniform velocity profile) does not represent the velocity distribution entering the main section of the wind tunnel during the experiments. In fact, experimental profiles in Figure 2a do not display a symmetrical shape in relation to the axis z = 0, presenting higher velocities next to the top; given that geometry is symmetrical, such asymmetric profiles can be regarded to a non-uniform velocity distribution in the inlet of the main section. Hudson (2009) also found an uneven velocity distribution in the UNSW wind tunnel and pointed that such asymmetry can result from the influence of the air conduction tube and the inlet duct. In such sense, the inlet boundary condition adopted represents the idealized inlet condition desired for the wind tunnel, which is not always obtained in the real situation. In the case of available experimental velocity measurements at the inlet, they could be used to implement an inlet boundary condition that would probably lead to results more suitable to the situation verified in the experiments. It has to be noted, however, that a not well-predictable velocity distribution inside the wind tunnel is not the desired situation, because, in such a case, the equipment behaviour is not characterized by a "nominal velocity" (Hudson, 2009).

The example discussed here suggestions challenging aspects of the experimental validation of CFD studies with enclosure sampling devices. The number of published works reporting experimental details and measurement results (e.g., velocity or concentration profiles, emission rates under controlled conditions, flow visualization) that can support a validation comparison is quite reduced. Furthermore, the wide variety in terms of design and operation settings makes it even more difficult to obtain experimental data that is suitable to be used in validation of a specific situation of interest. For example, in the present case, if the simulations of Lin et al. (2012) were repeated and validated against their experimental data (that are considerably detailed and useful for their case), it would not provide any confidence in respect to simulations of the UNSW wind tunnel, given the differences in terms of size and velocity magnitude. In a same manner, using data from turbulent-flow wind tunnels (as from Saha et al., 2011) would not be appropriate, because the UNSW wind tunnel presents a laminar flow. Considering these difficulties of adapting data from other studies, the solution normally is to conduct experiments specifically designed to provide validation (and boundary conditions) representative for each particular case.

However, in certain cases, CFD simulations may be intended to "anticipate" (this word has to be used with much regard) the behaviour of some device, which is a relatively frequent practice for preliminary design analysis in some fields of engineering. When, in these cases, there is no experimental data from similar situations that could provide validation, one can try to validate against ideal theoretical problems (with kwon analytical solution) which present some relation to the problem being studied – the level of confidence being directly dependant on how close the theoretical situation is to the simulated one. Comparison with theory, when possible, can also serve to complement experimental validation, as used by Lin et al. (2012), which compared their results with the analytical solution for developed laminar flow between two flat plates.
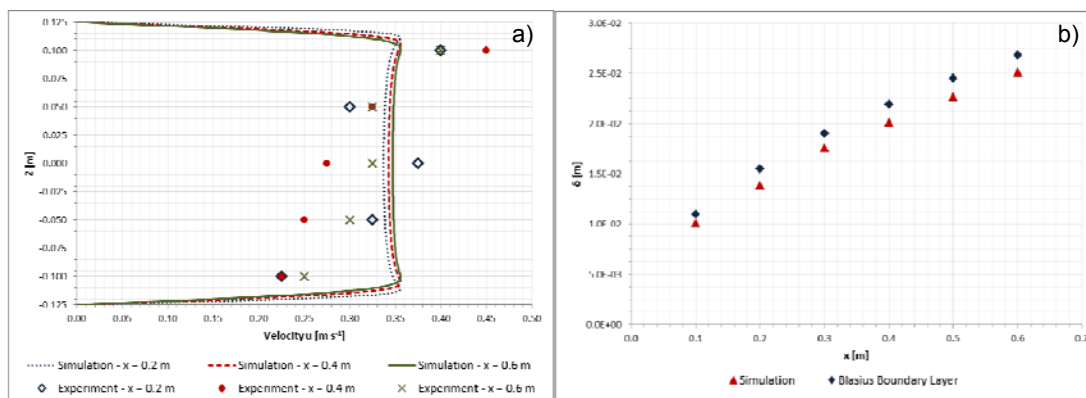
Figure 2: (a) vertical velocity profiles at longitudinal positions x = 0.2 m, x = 0.4 m and x = 0.6 m resulting from CFD simulation and experimental velocity values derived from Jiang (1993); (b) velocity boundary layer thickness (δ) from the simulations results and from the Blasius formulation.

At this point, it is interesting to analyse the relation among the experimental mass transfer results and the theoretical model that was used by Bliss et al. (1995) and the results of the present CFD simulation. In order to model the mass transfer coefficient (k_G) for ammonia inside the UNSW wind tunnel, Bliss et al. (1995) evocated the following equation:

$$k_G = \frac{0.664D}{L}\left(\frac{U\rho L}{\mu}\right)^{1/2}\left(\frac{\mu}{\rho D}\right)^{1/3} \tag{1}$$

Where: D is the molecular diffusivity ($m^2\ s^{-1}$) of the compound (ammonia); L is the length (m) of the boundary layer; U is the free stream velocity ($m\ s^{-1}$); ρ is the air density ($kg\ m^{-3}$); and μ is the dynamic viscosity ($kg\ m^{-1}\ s^{-1}$) of air.

This equation is obtained averaging (along the whole boundary layer extension) the local mass transfer coefficient for a laminar boundary layer with velocity profiles described by the classical solution of Blasius (which can be found, for example, in Schetz, 1984). For a temperature of 15 ℃, the equations proposed by McQuillan et al. (1984) for dry air give ρ = 1.226 $kg\ m^{-3}$ and μ = 1.797 × 10^{-5} $kg\ m^{-1}\ s^{-1}$ and Bliss et al. (1995) use ammonia diffusivity in air D = 2.017 × 10^{-5} $m^2\ s^{-1}$. With these values, taking U = 0.33 $m\ s^{-1}$ and considering that the boundary layer expands along the whole extension of the measurement section (L = 0.8 m), Eq(1) estimates a mass transfer coefficient k_G = 2.020 × 10^{-3} $m\ s^{-1}$. For the velocity of 0.33 $m\ s^{-1}$, the average of experimental values of Bliss et al. (1995) was k_G = 1.788 × 10^{-3} $m\ s^{-1}$, a difference in the order of 10 % from the theoretical value. According to the authors, this difference can be attributed to the precision limits of the analytical method used for ammonia quantification in the outlet air. It can be suggested that additional factors may also have contributed to this difference, in special: imprecision of the estimative of ammonia concentration adjacent to the gas-liquid interface (precise near-interface estimates of concentration are very challenging for compounds like ammonia), whose value was used to calculate the experimental k_G; insufficient recovery rate in the wind tunnel, once the experiments were carried out before the modifications introduced by Wang et al. (2001); and the distorted velocity profiles discussed above, which clearly do not follow exactly the premises of the Blasius boundary layer formulation.

The results of the CFD simulation also show a boundary layer over the gas-liquid interface that does not correspond strictly to the Blasius formulation. As can be seen in the profiles exhibited in Figure 2a, the maximum velocity that occurs at the edge of the boundary layer at each position is different from the velocity at the midpoint along the height of the wind tunnel (position z = 0), which here is supposed to play the role of the "free stream velocity". This effect comes from the conservation of mass (displacement of air in the vertical direction) while the boundary layer is in development. Interestingly, a similar effect can be observed in some of the experimental profiles reported in Saha et al. (2011). Weyburne (2010) points that such effect makes the pressure gradient in the flow direction at the boundary layer assume a non-zero value, deviating from an essential condition (zero pressure gradient) to derive the Blasius solution.

In Figure 2b, it is presented a comparison between the momentum boundary layer thickness obtained in the CFD simulation and the values calculated based on Blasius solution (Schetz, 1984). Up to a boundary layer length of 0.6 m, the profiles have fairly the same shape, being well described by a power equation (after the extension of 0.6 m, the boundary layer in the wind tunnel is greatly affected by the contraction zone). The boundary layer verified in the simulation presented a smaller thickness when compared to the Blasius solution (around 10 % thinner, at the maximum), as a result of the higher velocities at the edge. The average concentration gradient at the interface obtained from the CFD simulation can be used to calculate the ammonia emission rate and, consequently, the average mass transfer coefficient, resulting in k_G = 2.069 × 10^{-3} $m\ s^{-1}$. This value is slightly higher than the expected value from the theoretical estimate given by Eq(1), which is consistent with the mentioned higher velocities and thinner boundary layer thickness obtained in the simulation.

From the above discussion concerning to the relation between CFD results and the theoretical boundary layer model, it can be inferred that the simulation in fact was able to represent an ideal situation for the wind tunnel, also capturing a (expected) slightly difference in comparison with Blasius formulation. Such deviation is likely to occur in a real UNSW wind tunnel operating in near-ideal conditions (well distributed inlet air velocity). Even being small, this difference from the theoretical model has to be known and properly handled in practical situations. Another effect that can also exert a significant influence is the side-wall effect due to the three-dimensional geometry of the wind tunnel. This issue was not treated here, but Saha et al. (2011) present interesting insights about it.

4. Conclusions

The example discussed here illustrated the use of CFD technique to analyse a wind tunnel device for quantification of odorant emission at passive liquid surfaces. It showed the basic considerations that were made to support the definition of the computational domain, the numerical model and the boundary conditions, as well as the assumptions and simplifications involved. It has to be highlighted the importance of providing this type of information in as much detail as possible when reporting results from a CFD simulation; they will help in the interpretation of the results and comparison with other studies. Mesh sensitivity tests and validation are also very important to enhance the confidence over the obtained results. Challenging aspects of the experimental validation using data reported in published works were pointed. Comparison with calculations derived from the theoretical model of Blasius for the laminar boundary layer indicated that the results of the CFD simulation correspond to an ideal situation for the wind tunnel, which, nevertheless, slightly deviates from the Blasius formulation. It is necessary that such deviation is considered adequately in the interpretation of experimental results.

Acknowledgements

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