The use of CFD for the development of a field air pollution exposure system

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Abstract

Research on the effect of air pollutants on plants employs both laboratory and field experimental facilities. The advantage in using field-based facilities is the closer correlation of experiments with the natural environment. For field facilities, two distinct types of approach have been taken; (i) exclusion of ambient air in the experimental area and its replacement with air of the desired pollutant concentration using forced air delivery and various enclosing structures (Open Top Chambers, Air Exclusion Systems), and (ii) enrichment of ambient air with the pollutant gas and using ambient wind for dispersion (Free Air Carbon Dioxide Enrichment, Zonal Air Pollutant System).

The objective of the work reported here is to develop a system for the fumigation of low growing plants which minimises some of the disadvantages of the above systems, namely modification of the experimental environment (a problem with exclusion systems) and, for air enrichment systems, high costs and the lack of the facility to exclude background pollution.

Computational fluid dynamics (CFD) software has been used to calculate and visualise system performance of various design options. Comparisons with a to-scale laboratory model of one design showed reasonable agreement between measured and predicted values. It is seen that CFD is a useful tool to gain an understanding of the flow configurations and pollutant gas distribution in such systems and to optimise the system design.

1 Introduction

The effect of air pollutants on plants has been studied since the end of the 19th century. Early work was largely conducted in greenhouses and closed indoor chambers and this approach is employed up to the present day using controlled environment chambers. The recognition in the late 1960’s that plant physiological response to pollutants is very sensitive to environmental variables led to the development of field based systems which were intended to approximate more closely to natural conditions. Foremost among these systems are Open Top
Chambers (OTCs) which are still widely used (Fuhrer\textsuperscript{1}). An OTC consists of a circular open topped chamber with transparent walls placed over plants growing in the field, into which is pumped the pollutant gas, usually at the base of chamber. Although use of an OTC does improve the correlation with natural conditions, significant disadvantages remain particularly with respect to elevation of chamber temperature above ambient, reduced light levels and dilution of pollutant gas concentration due to the ingress of ambient air.

Efforts have been made to develop alternative field fumigation systems with the most prominent to date being Free Air Carbon Dioxide Enrichment (FACE) (Hileman et al.\textsuperscript{2}), Zonal Air Pollution (ZAP) (Runeckles et al.\textsuperscript{3}) and Air Exclusion (AE) systems (McLeod and Baker\textsuperscript{4}). The ZAP and FACE systems dispense with a containing structure and instead use ambient wind to disperse the pollutant gas over the experimental plot. Wind speed and direction is sensed and dispensing nozzles placed in the area are selectively opened under computer control. This approach is relatively successful but carries a high capital and running cost. Two inherent disadvantages are gradients in pollutant gas concentration across the plot and the site specific nature of results due to the presence of other gases in the ambient air. The latter presents a serious problem because without excluding ambient air, interactions of the pollutant under investigation with the unknown variety of pollutants in the ambient air makes interpretation of experimental results more difficult.

AE systems are less sophisticated in design but offer the potential for a cheaper and a less site specific system than FACE and ZAP. In an AE system plants are fumigated with air of controlled composition via tubes which are placed between plant rows in the experimental plot. The fumigation air may be filtered to simulate a clean environment but may also be enriched with pollutants after filtering to investigate the effect of any single pollutant or a composition of different pollutants while excluding the effects of background levels of pollutants at this specific site. Disadvantages of AE are unnaturally high wind velocities around the plants as the air jet is directed towards the canopy. They are very susceptible to dilution by ambient air; their efficiency varies with ambient wind speed. The systems are limited to low growing plants and the ducts between plant rows create a form of enclosing structure which can change the microclimate around plants.

The work reported here is directed towards the development of a Field Air Pollutant Exposure (FAPE) system for the exposure of low growing plants to ozone which combines advantages of FACE, ZAP and AE systems. Desired performance attributes of the system are low capital and operating costs, exclusion of ambient air to an acceptable degree and maintenance of a stable and even distribution of pollutant gas around plants in the experimental plot without changing the microclimate. Attainment of these attributes will require a design which optimises air flow and gas dispersion, and a control system similar to that used in FACE systems. The work reported here is concerned with the optimisation of the design aspects of the problem.
2 FAPE System Design Characteristics

The starting point for the design was existing AE systems which use ducts for fumigation of the plots. Any number of ducts may be placed in any configuration as long as the resulting structure does not adversely influence the plot microclimate. The open structure of the system limits the spacing of ducts and places the emphasis on attaining the maximum degree of air exclusion. Here we examine two configurations, rectangular and circular. Design variables considered are (i) number of ducts delivering into the plot, (ii) height of ducts above the soil surface, (iii) number and size of duct holes, (iv) location of duct holes, and (v) volume of air delivered to the plot.

Figure 1: Vertical section through a rectangular duct layout using two pipes.

Figure 1 shows the layout of a rectangular configuration using two ducts. It consists of a straight run of plastic pipe either side of a plot of width \(d\), at a height \(h\), running from a plenum supplying filtered air. Three rows of holes (diameter \(f\)) at angles of \(\alpha, \beta, \chi\) deliver the enriched air to the plot.

Figure 2: Vertical section through a circular duct layout using two pipe circles.

Figure 2 shows the layout of a circular design. It consists of two ring-shaped ducts of diameter \(d\), one at ground level and one at a height \(h\). The lower pipe has one row of holes of diameter \(f_1\) at an angle \(\alpha\), the upper duct has two rows of holes of diameter \(f_2\) at the angles \(\beta\) and \(\chi\) respectively.
3 CFD Model Construction

A finite element based computational fluid dynamics software (Fluid Dynamics Analysis Package, FIDAP 7.5, FDI, Evanston, IL, USA) running on a Sun Sparc 2000 was used to model the problem. Rectangular systems were set up as two dimensional. Circular designs were modelled as an axi-symmetrical problem. It was assumed that the two dimensional and axi-symmetrical solutions can give reasonable results although they do not fully represent the three dimensional nature of the problem. The solutions represent the outlet holes in the duct as a continuous slot rather than a discrete number of holes and therefore overestimate the average species concentration and the velocities in the domain. However, the objective at this stage of the CFD modelling was exploration of a range of design configurations and since the relative performance of each configuration could still be assessed the much greater time required to set up and solve three dimensional models was not justified.

3.1 Mesh generation

A characteristic of the models was the wide size range of system components, in particular the size of the duct holes in comparison to the size of the whole domain. In order to achieve the appropriate degree of accuracy in the region of the holes, a high gradient in element size was required, i.e. very small elements around the holes and large elements at the margins of the model. For this problem the standard $k$-$\varepsilon$ turbulence model was employed for which FIDAP uses special near-wall elements. These wall elements are those close to rigid walls and special equations for the laminar boundary layer are used. These equations are only applied to the elements in the direct vicinity of walls and therefore these elements must be thick enough to contain the whole laminar boundary layer. FIDAP provides two different mesh types, mapped and paved. Mapped meshing is regular meshing constructed by drawing lines connecting opposite mesh edge points. It is limited to four sided regions and the geometry has to be decomposed into suitable areas. Paved meshing is an automatic process applicable to almost any geometry. An example of the mesh resulting from these considerations can be seen in Figures 3 and 4. Both techniques were used to generate the mesh for the discussed models as shown in Figure 4.

3.2 Boundary Conditions

All models were calculated as incompressible as the highest velocity was 10 m/s and the Mach number was far below the critical value for this simplification. They were regarded as isothermal as temperature gradients in the field system were negligible. These assumptions cut computing time and CPU requirements considerably.

There were no restrictions applied to any degree of freedom to the left and top margins of the models (as shown in Figure 1 and 2) as this was the border of the computational domain in the open air. Symmetry boundary conditions were applied to the right hand edge of the domain by setting the x-components of the velocity to
zero in rectangular models or setting the radial component of the velocity to zero in circular models. The bottom edge is the soil surface where both velocity components were set to zero. Both velocity components were set to zero at the duct’s inner and outer surface.

A pressure boundary condition was applied inside the ducts. In preliminary test runs it was shown that the placement of the pressure boundary condition in the duct does not have any significant influence on the performance of the exiting air jets as long as this pressure boundary condition is placed more than two hole diameters away from the outlet holes. For simplicity, a pressure boundary condition was then applied to a section of boundary in the tube remote from the exit holes.

Values of air density and viscosity at sea-level and ambient temperature were applied to the whole domain. Gradients in density and viscosity due to gradients in species concentrations were neglected since the maximum of 200 ppb of pollutant gas was not significant. The molecular diffusivity was set to 1.0 E-5 m²/s.

3.3 Solution Process

The solution of the system of equations was calculated in two stages. In the first stage, the equations of continuity, motion, turbulent kinetic energy \( (k) \) and dissipation rate of turbulent kinetic energy \( (\varepsilon) \) were solved providing results for the velocity vector \( \mathbf{v} \) field, the pressure field, the \( k \)-field, and the \( \varepsilon \)-field. In the second step the concentration of filtered air was calculated by making use of the turbulent Schmidt number \( S_t \), which links turbulent diffusivity \( D_\varepsilon \) and turbulent viscosity \( \mu_\varepsilon \) such that

\[
D_\varepsilon = \frac{I}{S_t} \cdot \frac{\mu_\varepsilon}{\rho}
\]

where \( \rho \) is the gas density. The turbulent viscosity is calculated from \( k \) and \( \varepsilon \) so that \( D_\varepsilon \) can be expressed as

\[
D_\varepsilon = \frac{I}{S_t} \cdot C_\mu \cdot \frac{k^2}{\varepsilon}
\]

where \( C_\mu \) is a constant in the k-\( \varepsilon \) turbulence model and was set to the default value of 0.09 (Zannetti\(^5\), Wilcox\(^6\)). The turbulent Schmidt number was assumed to be constant, \( S_t = 0.9 \), a value which has proved to be appropriate for most flow simulations (Fluid Dynamics International\(^7\)). Therefore, given the \( \mathbf{v} \)-field, the \( k \)-field, the \( \varepsilon \)-field and the value for molecular diffusivity, the concentration of filtered air can be calculated in the second stage of the solution process. This step by step solution is only possible by assuming that the species concentration does not affect density or viscosity of the fluid.
4 Results and Discussion

4.1 Simulation

The design variables used in the results shown here are $h = 500$ mm, $d = 1600$ mm, $f = 10$ mm, $\alpha = 90^\circ$, $\beta = 110^\circ$, and $\gamma = 180^\circ$ for the rectangular model, and $h = 350$ mm, $d = 1400$ mm, $f_1 = f_2 = 10$ mm, $\alpha = 90^\circ$, $\beta = 110^\circ$, and $\gamma = 20^\circ$ for the circular model. The diameters of the fumigation ducts were chosen according to commercially available ducting material and was 160 mm for the rectangular system and 100 mm for the circular system. Solutions were calculated for a 6 Pa pressure boundary condition in the tubes, equivalent to 3.2 m/s maximum hole exit velocity and a species concentration boundary condition of $c = 1$ in the ducts. Results presented here are constrained to a no ambient wind condition.

A speed contour diagram is shown in Figure 5 and 7 for the rectangular and the circular system respectively. Figure 6 and 8 show the calculated concentration of filtered air in the plot for the rectangular and the circular system respectively.

In the rectangular system, a mirrored "mixing vortex" provides for good mixing of air which leads to a relatively even concentration of filtered air in the planting area. The lower row of holes contributes very little to the flow situation in the plot. The air from the lower holes streams away from instead of into the system. This situation may be undesirable as this disturbs the flow pattern in neighbouring plots. The concentration of filtered air is relatively low (40%) as the system is not sufficiently isolated from ambient air.

In the circular system, the lower duct ring supports the mixing vortex in the system. This results in a better mixing and more even concentration of filtered air in the plot. The system is well protected against ingress of ambient air as the two upper jets blow a considerable amount of air out of the system. The circular system achieves therefore a higher concentration of filtered air (80%) in the plot and at the same time leaves the surrounding plots almost unaffected.

Figure 3: The FE-mesh for the rectangular system.
Figure 4: Mesh detail at a duct exit hole.

Figure 5: Speed contour of the rectangular system for $p = 6$ Pa, velocities in [m/s].

Figure 6: Concentration of filtered air in the rectangular system for $p = 6$ Pa and a species concentration boundary condition of $c = 1$ in the ducts.
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Figure 7: Speed contour of the circular system for $p = 6$ Pa, velocities in [m/s].

Figure 8: Concentration of filtered air in the circular system for $p = 6$ Pa and a species concentration boundary condition of $c = 1$ in the ducts.

Figure 9: Measured velocity vector in the rectangular system for $p = 6$ Pa.
4.2 Validation

An experimental laboratory model of the rectangular system on a 1:1 scale (in the plane shown in figure 1) was used to investigate the accuracy of the CFD model. The pipe length in the axial direction was 1 m running orthogonally from a wall. All measurements were taken at points in a vertical plane 0.5 m from the wall. Air velocity was measured using a hot wire anemometer; the sensor was oriented parallel to the flow direction previously determined using a smoke tracer. Measurements were taken in a square grid of 50 mm spacing. Pressure was measured inside the pipes using a pitot tube connected to a micromanometer. Air flow rate was set by adjusting air pressure in the pipe to 6 Pa which resulted in a mean hole exit velocity of 2.15 m/s which compares well with the predicted value of 2.28 m/s.

A plot of measured velocity vectors is shown in Figure 9. The general flow pattern is similar in shape to that predicted for the rectangular model (Figure 5). In particular, the mixing vortex predicted by the CFD model was observed. However measured velocities in the domain outside the pipes were approximately 30% lower than the calculated values. This can be explained by the error inherit in using a two dimensional model for this problem as explained earlier. Although a greater density of measurement points and more precise determination of flow direction would be required to properly validate the CFD model, the experimental results suggest that the CFD model is capable of a close approximation to the physical system.

5 Conclusions

The performance of FAPE system prototypes were investigated by means of a CFD-software package. CFD is shown to be a useful tool for the development of experimental fumigation systems where the flow pattern of fumigating air and distribution of pollutant concentration is critical to production of useful research data. It helps in determining promising design approaches and providing information for the understanding of flow configurations in fumigation facilities. The influence of a large number of design parameters can be checked relatively easily and performance characteristics can be visualised. A simple system configuration was experimentally validated with good correlation between predicted and measured values. This leads to a degree of confidence in the application of CFD to more complex designs.

The importance of good design for fumigation systems is emphasised in the results of the CFD simulations. As the two examples presented here show clearly, changing the plot shape and the orientation of the jets delivering filtered or enriched air to the plot can change system performance considerably. Filtered air concentrations in the planting area were shown to be strongly dependent on the number and orientation of the exit holes. The effect of free jets may result in the sucking in rather than exclusion of ambient air. The modelling also indicates that even in static ambient conditions interference between plots must be considered.
The use of a secondary delivery pipe, as examined in the circular model, can improve both the plot exclusion rate and the degree of insulation from neighbouring plots.

The results presented here show that CFD modelling provides a valuable tool for exploring FAPE system design options. Further work is required to investigate the effect of various ambient wind profiles on system performance. Selected designs will then be evaluated in the field and the appropriate level of system control determined.

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