Odour Source Identification in a Complex Flow Environment using a Particle Trajectory Model

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Introduction

• The need has arisen to identify potential odour emission sources from boundary monitoring.

• More often than not, airflow in industrial situations is subject to interference from structures.

• Popular trajectory models used (e.g. HySplit) cannot accurately depict particle motion in complex flow situations.

• In addition, the temporal resolution of the data often used in the trajectory model is too coarse to resolve the flow in these situations.

• A new pseudo 3D model based on the Navier Stokes equations, is presented here.
Navier Stokes Equations

- These are equations which can be used to determine the velocity vector and pressure field that applies to a fluid, given some initial conditions.

- Developed from Newton’s second law.

\[
\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{\nabla P}{\rho} + \nu \nabla^2 \mathbf{u}
\]

- The above equation is too difficult to solve analytically.

- Approximations and simplifications to the equation set have been made until they had a group of equations that they could solve using a variety of techniques like finite differencing.
Navier Stokes Equations

• The flows are characterised by a system of non-linear PDEs (in 2D component form):

Momentum equations:

\[
\frac{\partial u}{\partial t} + \frac{\partial p}{\partial x} = \frac{1}{Re} \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) - \frac{\partial (u^2)}{\partial x} - \frac{\partial (uv)}{\partial y} + g_x
\]

\[
\frac{\partial v}{\partial t} + \frac{\partial p}{\partial y} = \frac{1}{Re} \left( \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right) - \frac{\partial (uv)}{\partial x} - \frac{\partial (v^2)}{\partial y} + g_y
\]

Continuity equation:

\[
\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0
\]
Numerical Treatment (time stepping)

\[ u^{(n+1)} = F^n - \delta t \frac{\partial p^{(n+1)}}{\partial x} \]  \hspace{1cm} (1a)

\[ v^{(n+1)} = G^n - \delta t \frac{\partial p^{(n+1)}}{\partial y} \]  \hspace{1cm} (1b)

where

\[ F = u^n + \delta t \left[ \frac{1}{Re} \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) - \frac{\partial (u^2)}{\partial x} - \frac{\partial (uv)}{\partial y} + g_x \right] \]  \hspace{1cm} (2a)

\[ G = v^n + \delta t \left[ \frac{1}{Re} \left( \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right) - \frac{\partial (uv)}{\partial x} - \frac{\partial (v^2)}{\partial y} + g_y \right] \]  \hspace{1cm} (2b)
Discretization

• The derivatives in Eq^n. 2a and 2b are discretised in two dimensions using finite differencing:

\[
\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = \frac{u(x_{i+1,j}) - 2u(x_{i,j}) + u(x_{i-1,j}) + u(x_{i,j+1}) - 2u(x_{i,j}) + u(x_{1,j-1})}{\delta y^2}
\]

\[
\frac{\partial (uv)}{\partial y} = \frac{1}{\delta y} \left( \frac{(v_{i,j} + v_{i+1,j})}{2} \frac{(u_{i,j} + u_{i,j+1})}{2} - \frac{(v_{i,j-1} + v_{i+1,j-1})}{2} \frac{(u_{i,j-1} + u_{i,j})}{2} \right)
\]

\[
\frac{\partial (u^2)}{\partial x} = \frac{1}{\delta x} \left( \left( \frac{u_{i,j} + u_{i+1,j}}{2} \right)^2 - \left( \frac{u_{i,j-1} + u_{i,j}}{2} \right)^2 \right)
\]
Discretization

Pressure is determined by solving:

\[
\frac{\partial^2 p^{(n+1)}}{\partial x^2} + \frac{\partial^2 p^{(n+1)}}{\partial y^2} = \frac{1}{\delta t} \left( \frac{\partial F^{(n)}}{\partial x} + \frac{G^{(n)}}{\partial y} \right)
\]  

(3)
Boundary Conditions

• Fluid flows freely in the horizontal direction in from the boundary and out of the opposite boundary

• The vertical velocity approaches zero at the boundaries.

• Apply no-slip boundary conditions to cells that are adjacent to internal obstacle cells. This forces the u and v velocity to tend towards zero in these cells.
Calculation Methodology

Determine building locations/heights. Apply no-slip boundary conditions

Define inflow conditions (u and v components)

Write u, v and w fields for level

Compute new velocity field $u^{(n+1)}$ and $v^{(n+1)}$ from $p^{(n+1)}$ using eqn 1a and 1b

Compute $F^{(n)}$ and $G^{(n)}$ from $u^{(n)}$ and $v^{(n)}$ using eqn 2a and 2b

Solve the Poisson equation for pressure $p^{(n+1)}$ using eqn 3

$$F = u^n + \delta t \left[ \frac{1}{Re} \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) - \frac{\partial(u^2)}{\partial x} - \frac{\partial(uv)}{\partial y} + g_x \right]$$

$$G = v^n + \delta t \left[ \frac{1}{Re} \left( \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right) - \frac{\partial(uv)}{\partial x} - \frac{\partial(v^2)}{\partial y} + g_y \right]$$

$$u^{(n+1)} = F^n - \delta t \frac{\partial p^{(n+1)}}{\partial x}$$

$$v^{(n+1)} = G^n - \delta t \frac{\partial p^{(n+1)}}{\partial y}$$

(Next level)

(If solution converges then)

(Multiple iterations)
Defining Buildings

- No obstacle
- Obstacle height defined spatially
Wind Vectors
Vertical Velocity
Particle Trajectories

• 3D kinematic trajectory model (D’Abreton, 1996; D’Abreton and Tyson; 1996).

• The model is Lagrangian, with motion being described in terms of air parcels moving with air streams.

• The model uses the explicit method of integration:

\[ x(t+dt) = x(t) + V[x(t)]dt \]

• The parcel velocity vector \( V = (u, v, w) \) is the sum of the mean and turbulent component

\[ V = \bar{V} + V' \]
Particle Trajectories

• Spatial fields of flow (u-, v- and w-components) are used to drive the particle trajectory model

• For the dispersion calculations the turbulence components are derived from the definition of the TKE

• The relationship between the horizontal and vertical components is explicitly defined through the turbulence anisotropy factor:

\[
\frac{W'^2}{U'^2 + V'^2}
\]
Particle Trajectories

- Particles transported upward higher than the mixing height at that location are reflected downward from the mixing height.

- Particles impacting on buildings are also reflected.
Examples
Examples
Conclusions

• This model allows near real-time solution of complex flow from a single onsite weather station.

• The complex flow model can be used the drive a particle trajectory model to determine near-field transport in disturbed flow.

• The example shows that in most cases, odour sources can be identified from a combination of trajectories. In particular, offsite odour sources can be identified, thereby averting the need for mitigatory actions and even potential legal issues.