Inverse prediction of contaminant transport in enclosed environment

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Outline

- Background of inverse modeling
- Quasi-reversibility (QR) method
- Application 1: QR method for a 2-D aircraft cabin
- Application 2: QR method for a 3-D office with displacement ventilation
- Conclusions
Background: Inverse problems

Inverse problems are ill-posed

A problem that does not satisfy any of the following terms is ill posed

(1) The solution exists; (2) The solution is unique;
(3) The solution is stable
Background: Strategies to handle inverse problems

- **Existence** – Accurate initial conditions
- **Uniqueness** – Sufficient prior information to make the solution unique
- **Stability** – Solving modified equations instead of the governing equations to improve stability
Background: Existing methods for inverse problems

- Analytical solution
- Optimization approach
- Probabilistic approach
- Direct approach

One solves the governing equation reversely with regularization or stabilization techniques
Background: Quasi-Reversibility method

The governing equation for a gaseous contaminant transport (without source):

\[
\frac{\partial \phi}{\partial \tau} + \frac{\partial}{\partial x_i} (u_i \phi) = \frac{\partial}{\partial x_i} \left( \frac{\Gamma}{\rho} \frac{\partial \phi}{\partial x_i} \right)
\]

The governing equation is unstable if it is solved reversely.

To improve the solution stability, replacing the second-order diffusion term with a fourth-order term:

\[
\frac{\partial \phi}{\partial \tau} + \frac{\partial}{\partial x_i} (u_i \phi) = \epsilon \frac{\partial^4 \phi}{\partial x_i^4}
\]

where \(\epsilon\) is the stabilized constant and an optimal \(\epsilon\) should be found.
QR method: Analysis of the discretized governing equation

The control volume in a 1-D flow

\[ \phi_p(\tau + \Delta \tau) = \frac{u_w \Delta \tau}{\Delta x} + \frac{\Gamma \Delta \tau}{\rho(\Delta x)^2} \phi_w(\tau + \Delta \tau) + \frac{\Gamma \Delta \tau}{\rho(\Delta x)^2} \phi_e(\tau + \Delta \tau) + \frac{1}{1 + \frac{u_e \Delta \tau}{\Delta x} + \frac{2 \Gamma \Delta \tau}{\rho(\Delta x)^2}} \phi_p(\tau) \]

Greater than one

Note: \( \Delta \tau < 0 \) in the inverse simulation

The above equation is unstable and unbounded with neighboring cells
QR method: Analysis of the discretized QR equation

\[ \phi_p(\tau + \Delta \tau) = \frac{\varepsilon \Delta \tau}{\Delta x^4} \phi_{WW}(\tau + \Delta \tau) + \frac{4 \varepsilon \Delta \tau}{\Delta x^4} - \frac{u_e \Delta \tau}{\Delta x} \phi_W(\tau + \Delta \tau) + \frac{4 \varepsilon \Delta \tau}{\Delta x^4} - \frac{u_e \Delta \tau}{\Delta x} \phi_E(\tau + \Delta \tau) + \frac{\varepsilon \Delta \tau}{\Delta x^4} \phi_{EE}(\tau + \Delta \tau) + \frac{1}{1 - \frac{6 \varepsilon \Delta \tau}{\Delta x^4} + \frac{u_e \Delta \tau}{\Delta x}} \phi_p(\tau) \]

With appropriate \( \varepsilon \), the above equation can be stable. However, it is not the CFD governing equation.
Application 1: QR method for a 2-D aircraft cabin

- Unstructured meshes
- Isothermal conditions
- A contaminant source at the floor level

RNG \(k-\varepsilon\) model with the second-order upwind scheme

- High velocity air around cabin walls
- Two vortexes were created
Application 1: Simulation schematics and initial concentration field

Simulation schematics

The contaminant concentration field at $t=6.0$ s
Application 1: Contaminant transport from $t=6$ s to $t=0$ s
Application 1: Comparison between inverse and forward modeling

The concentration field at $t=0.04$ s from the inverse modeling

The contaminant source location can be identified, however the strength is very dispersive

The concentration field at $t=0.04$ s from the forward modeling
Application 1: Contaminant concentration field at t=-2 s

A sensor at the left outlet would measure something if this concentration field is a possible scenario.

Otherwise, the inverse simulation should be stopped before t=-2 s.

The concentration field at t=-2 s

<table>
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<th>C</th>
<th>2.00E-04</th>
<th>1.15E-03</th>
<th>2.10E-03</th>
<th>3.05E-03</th>
<th>4.00E-03</th>
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Application 1: Initial and boundary conditions for 16 s inverse simulation

The forward concentration field at t=16 s

The contaminant exhausted out of the cabin should be added back as boundary conditions when doing the inverse simulation.

The forward concentration over time at two outlets
Application 1: Contaminant transport from $t=16 \text{ s}$ to $t=0 \text{ s}$
Application 1: Comparison between 16 s and 6 s simulation

The longer the simulation time, the more dispersive the results
Application 2: 3-D office with displacement ventilation

Geometry of an office (4ACH)

In this case, the role of diffusion is as important as convection.
Application 2: Initial concentration field at $t=32$ s

The contaminant concentration fields at $t=32$ s from the forward modeling will be used as the initial conditions to do the inverse study.
Application 2: Contaminant concentration fields at $t=0.04$ s

The results in the office are much poorer than those in the aircraft cabin because convection is not dominant.
Conclusions

- The QR method can identify contaminant source locations, however the strength is dispersive.
- The longer the simulation time, the more dispersive the results.
- The QR method requires the distribution of airflow, a contaminant concentration field, and boundary conditions.
- The QR method works better for the convection dominant flows.