# Transport of Pollutants Through Liquid-Gas Interfaces – a Numerical Approach

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**NIOSH-ERC**

**10th Annual Pilot Research Project (PRP) Symposium**

**October 1-2, 2009**

# OUTLINE

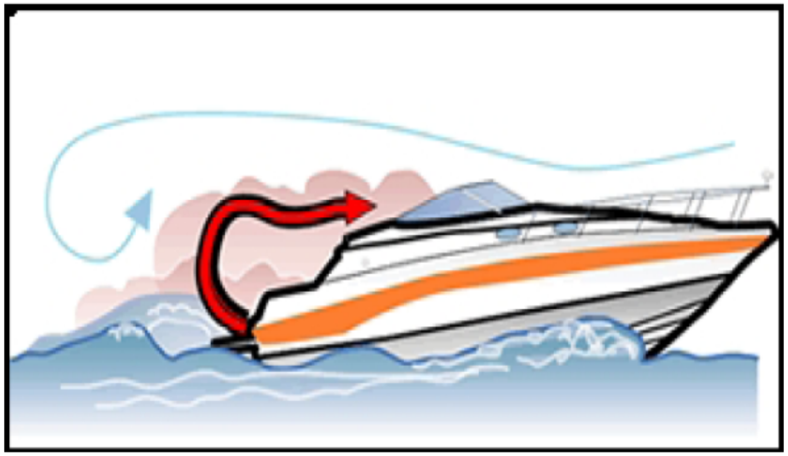
- Motivation
- Objectives of Present Study
- Problem Description
- Steps in Solution Procedure
- Results
- Future Work

# MOTIVATION

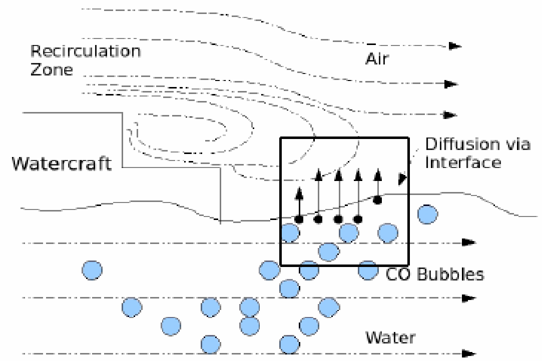
## MOTIVATION:

- Carbon Monoxide (CO) is ejected in the exhaust of combustion-based systems, e.g., watercraft.
- Being lighter than water, CO rises to water surface behind boat,
- Gets entrained into the cabin due to "Station-Wagon effect".
- Tests conducted by NIOSH show high CO concentration in back deck and cabin.
- Marine workers are exposed to high concentration of CO – higher than Immediately Dangerous to Life and Health (IDLH) value of 1200 ppm.

**Station-Wagon effect, *Courtesy: www.boat-ed.com***



**Transport of CO in water and across water-air interface**




## PREVIOUS RESEARCH CONDUCTED AT CFDRL:

- Studied dispersal of exhaust gases under the hull of a watercraft by modeling the water surface as a slip boundary.
- Effect of free surface on exhaust dispersal was not considered.

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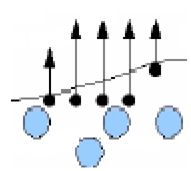
# OBJECTIVES

- Understand the flow physics involved in the transport of pollutants through an air-water interface.
- Develop a Computational Fluid Dynamics (CFD) model to simulate this flow physics.
- Accurately predict pollutant transport into air above the water surface by considering a unit process involving the pollutants and the air-water interface.



# PROBLEM DESCRIPTION

- Cylindrical vertical column:
  *Height*: 2m
  *Diameter*: 0.2m.

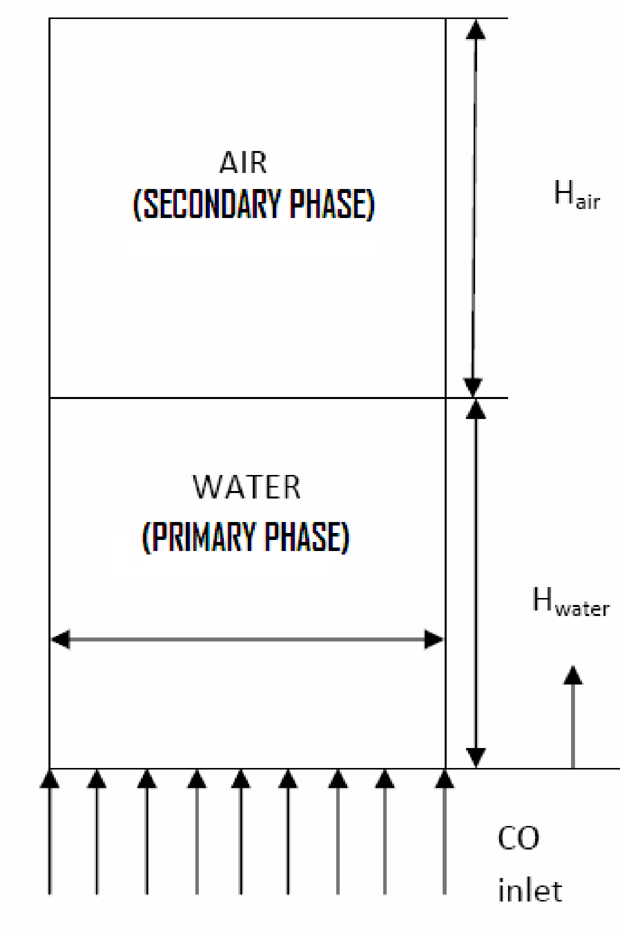
- Static height of water column:
  $H_{water}$: 1m.

- Mixture composition at inlet:
  *Volume Fraction of CO*: 0.5
  *Volume Fraction of Water*: 0.5

- CO bubbles, of diameter of 0.5 cm, flow in through the bottom, with a velocity of 0.1 m/s.

- Atmospheric pressure at top of air column.

Schematic of simulation domain



# STEPS IN SOLUTION PROCEDURE

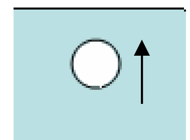
- Unsteady Incompressible Navier-Stokes equations are solved.

- Eulerian Multiphase model is used, treating phases as interpenetrating continua.

  *Primary phase*: Water

  *Secondary phases*: Air and CO

- "Virtual mass effect" term included in the momentum equations for both phases – accounts for inertia of primary-phase mass encountered by the accelerating bubbles.



- Schiller-Naumann drag model is used. In definition of $C_D$ , the Reynolds number uses the magnitude of the velocity of the primary phase relative to that of the secondary phase. Acceptable for use with all fluid-fluid pairs.

- Turbulence is modeled using the mixture *k-ε* equations.

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# STEPS IN SOLUTION PROCEDURE (Cont'd)

- **Pressure-velocity coupling is achieved using the Phase-coupled SIMPLE algorithm.**
  - **Velocities are solved coupled by phases, but in a segregated fashion.**
  - **Pressure correction based on *total volume continuity*.**
- **Second-order upwind scheme is used to discretize convection terms.**
- **The finite-volume flow solver FLUENT is used.**
- **Grid in r and z directions: 30x300.**
- **Time step: 0.0001 seconds.**
- **The solution at each time-step is assumed converged when scaled residuals of continuity and momentum conservation equations reach the order of $10^{-3}$.**
- **Simulation is continued until CO exits the column, i.e., for approximately 48 seconds.**

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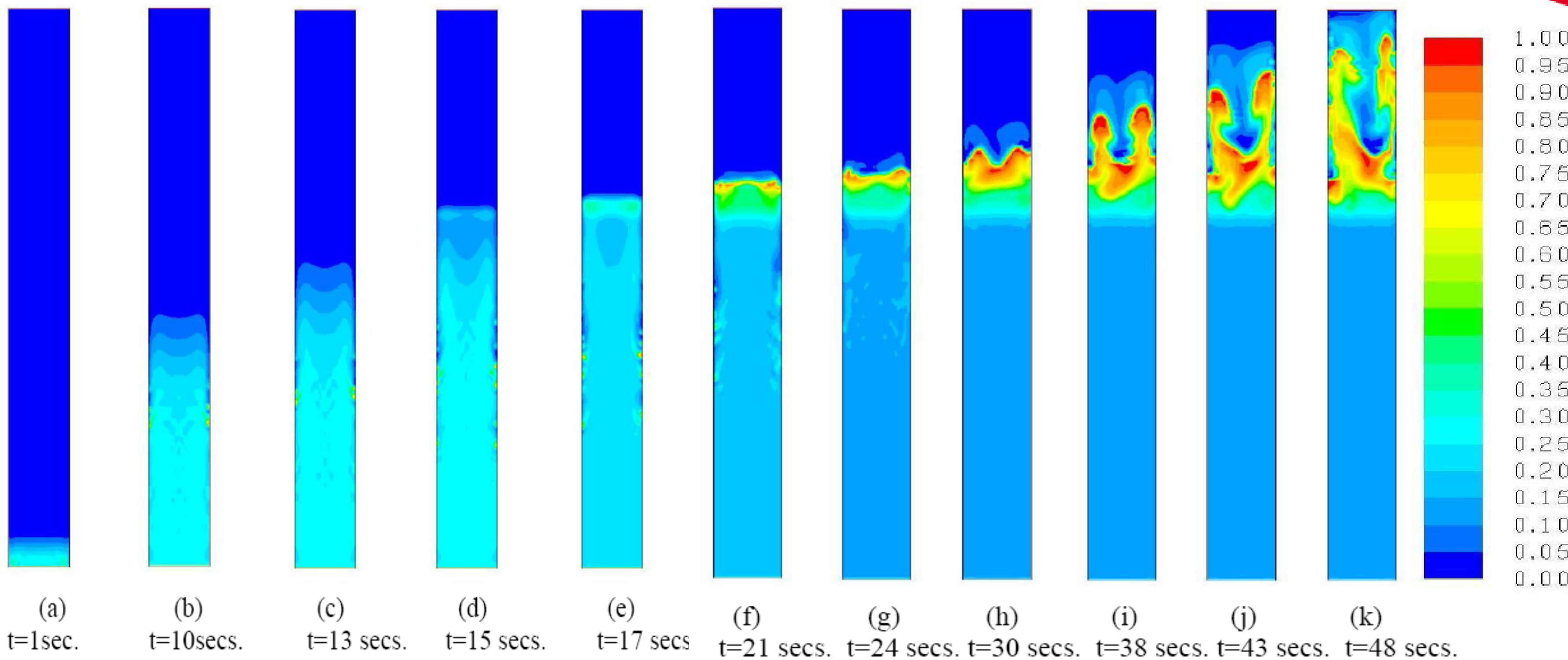
# RESULTS

**Transient CO motion along the vertical column**




**Key observations about CO behavior:**

- **CO gas enters in the form of bubbles, and rises to air-water interface.**
- **CO gas traverses water domain in approx. 15 secs to reach the air-water interface, owing to substantial driving force.**
- **Slow dispersal of CO in the air; CO takes approx. 35 secs to reach top of air column.**

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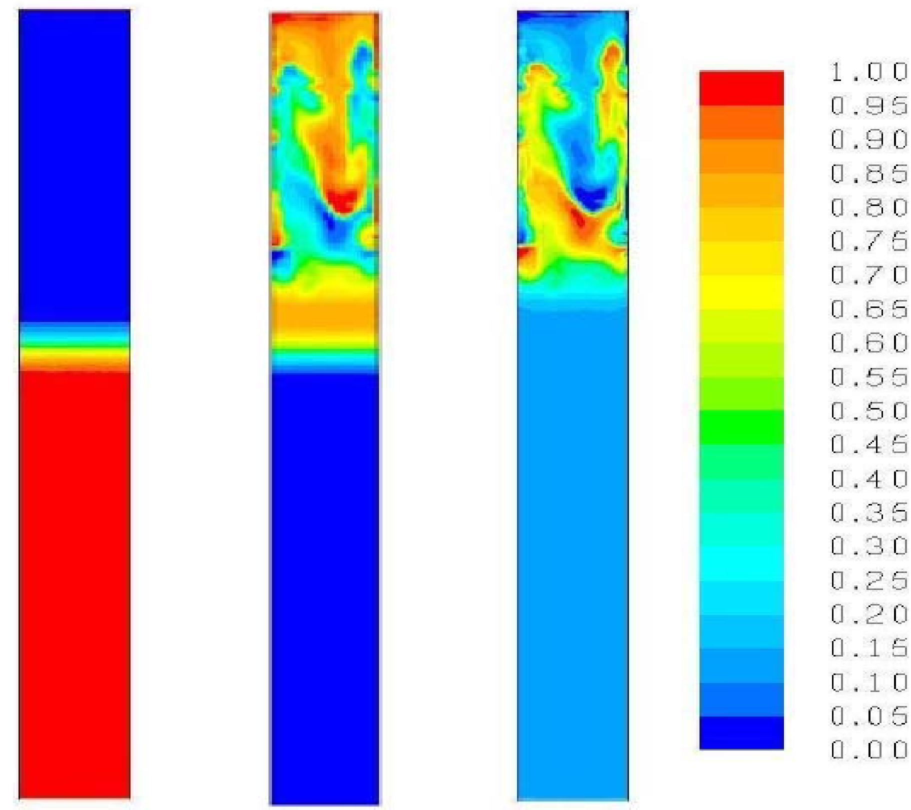
# RESULTS (Cont'd)

## General Observations about Air, Water and CO Volume Fractions

**Volume Fraction Contours at t=48 seconds.**




(a) Water, (b) Air, (c) CO

- **Rapid CO dispersal in water domain:**
  - ***Large density difference*** **: CO is 1000 times lighter than water.**
  - ***Initial momentum*****.**
- **Fractional increase in the level of the air-water interface as CO-water mixture enters the vertical column.**
- **CO bubbles rupture at air-water interface, and CO gas is freely dispersed into air region.**
- **Slow dispersal of CO in air domain:**
  - ***Milder density difference:*** **CO is only marginally lighter than Air.**
  - **Loss of initial momentum due to liquid drag.**

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# CONCLUSIONS

- ***Rapid CO movement through water domain* – due to initial momentum and large density difference between water and CO gas.**

- ***At the air-water interface* – CO bubbles rupture, and CO gas is freely dispersed into the air.**

- ***Milder density difference in the air domain* – much slower dispersal rates compared to CO movement in the liquid region.**

- **Air-water interface inadequately resolved.**

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# FUTURE WORK

- **Enhance *problem geometry* to include a watercraft and its surrounding environment.**
- **Devise methodology to adequately capture the air-water interface.**
- **Explore methods to capture *wave motion* at the air-water interface*, and the corresponding effect on the motion of the gas crossing the interface*.**

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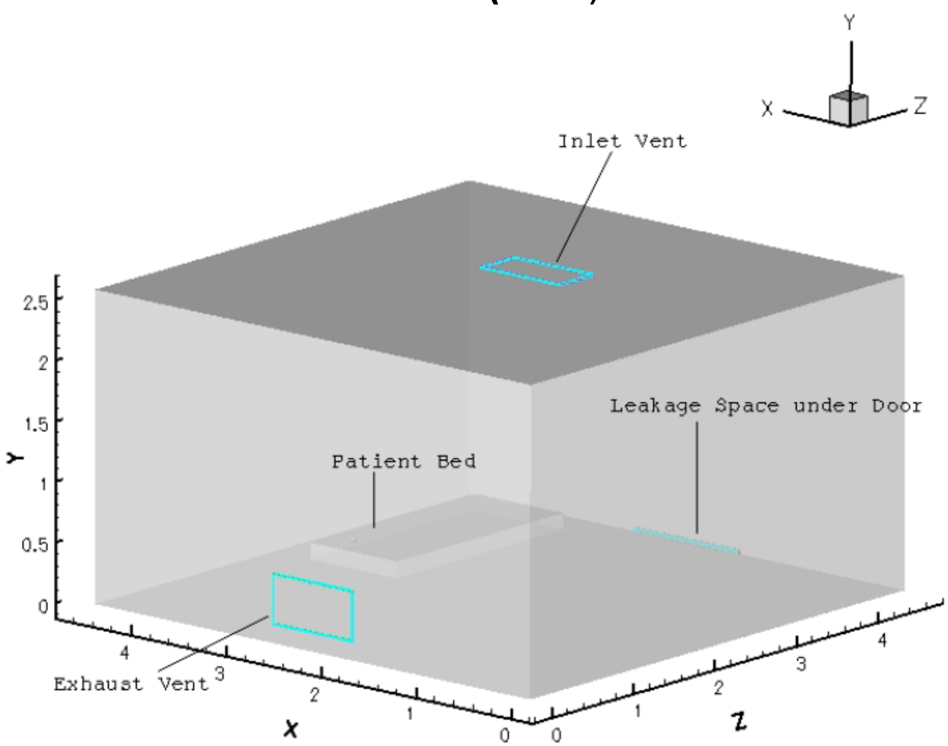
# HOW DID PRP HELP US?!

## KEY OUTCOMES:

- **Developed a deeper understanding of Multi-phase and Multi-species flow phenomena.**
- **Extended the use of Computational Fluid Dynamics to applications in Environmental Health and Occupational Safety.**

**Numerical Simulation of Pandemic Flu Dispersal in an Airborne Infection Isolation Room (AIIR)**

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# ACKNOWLEDGEMENTS


- National Institute for Occupational Safety and Health (NIOSH), Cincinnati, Education and Research Center (ERC).

- Dr. Amit Bhattacharya, Environmental Health, College of Medicine, UC.

- ERC Staff.

PRPS
pilot research project symposium

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# 10th Annual
# Pilot Research Project
# Symposium
## October 1-2, 2009

## Main Menu

Hosted by: The University of Cincinnati Education and Research Center Supported by: The National Institute for Occupational Safety and Health.
(NIOSH) Grant #: T42/OH008432-05



Produced by Kurt Roberts Department of Environmental Health