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Estimating fugitive emission of volatile organic compounds from evaporation ponds

Pouya Hadavi, Mohammad Safavi, Ali Parchamdar, Khosro Ashrafi, Ali Moosavi, Farhad Saffarian, **Mohammad Arhami**

EPA International Emissions Inventory Conference

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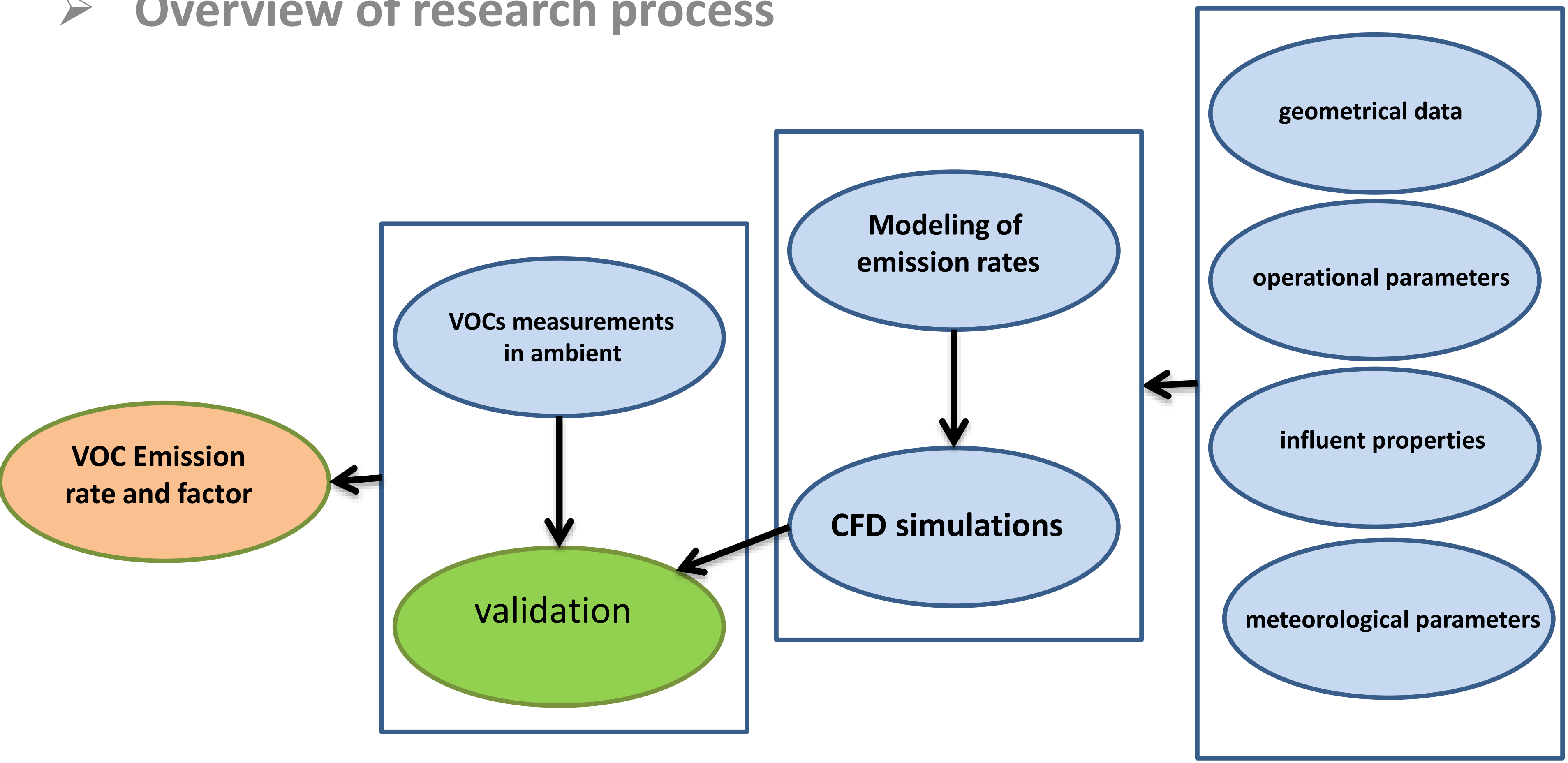
- Introduction
- Methodology
  - Measurement campaign
  - Emission model
  - 3D CFD model
- Results
  - Measurement
  - Simulation
  - Emission rate

Evaporation ponds

- O&G production
- Disposing produced water and other waste water
- Reduction of the disposing water (long term)
- Reducing oil component concentration (injection to the environment)
- Emission Volatile organic compounds (VOCs) from ponds surface

- **Evaporation ponds is favorable in this region**
  - High O&G production
  - Solar energy
  - High-efficiency
  - Very cheap
  - No additives
  - No extra energy

Overview of research process



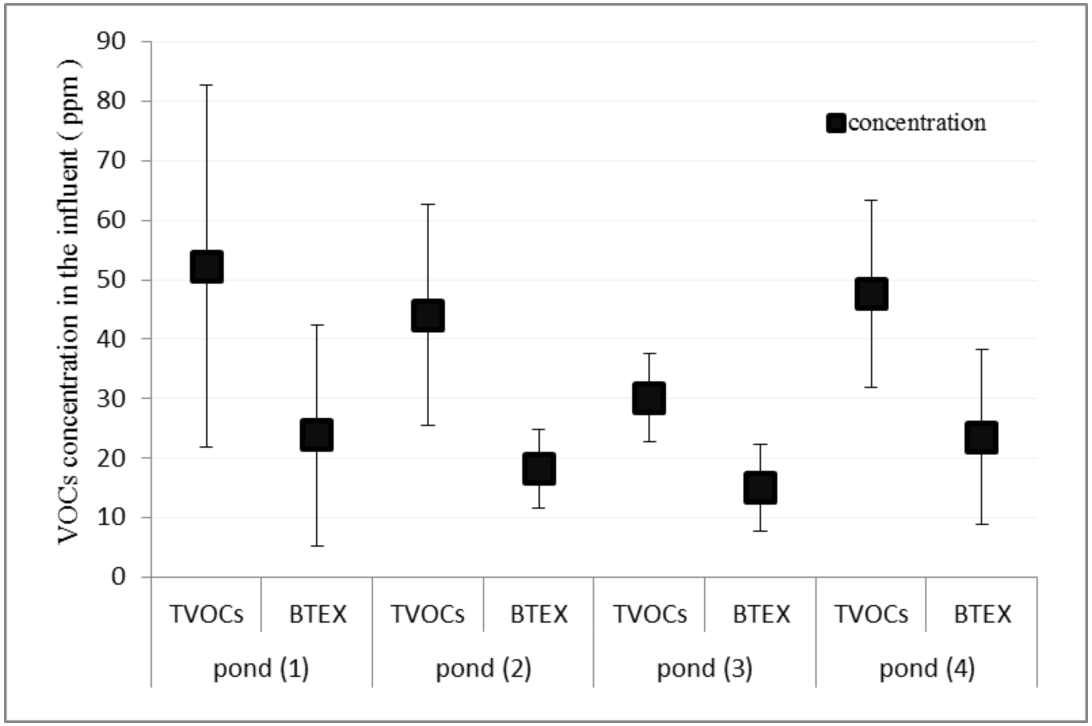
➢ Sampling and Measurement Campaign

- Samples and measurements were taken at 4 ponds
- Concurrent Measurements:
  - ✓ Pond Influent
  - ✓ Ambient
  - ✓ Meteorological parameters
- 4 sampling campaign for each pond
- Total of 16 measurement campaigns
- Measurements performed during one year (2015-2016)
- Each campaign period were about 2 weeks

Sampling and Measurement

- Influent water sample
  - VOCs and its speciation
  - BTEX
- Meteorological parameters
  - Wind speed
  - Wind direction
  - Temperature
- VOCs concentration in air
  - Around the pond
  - 3, 6 and 9 meters Above the surface
  - VOC Speciation

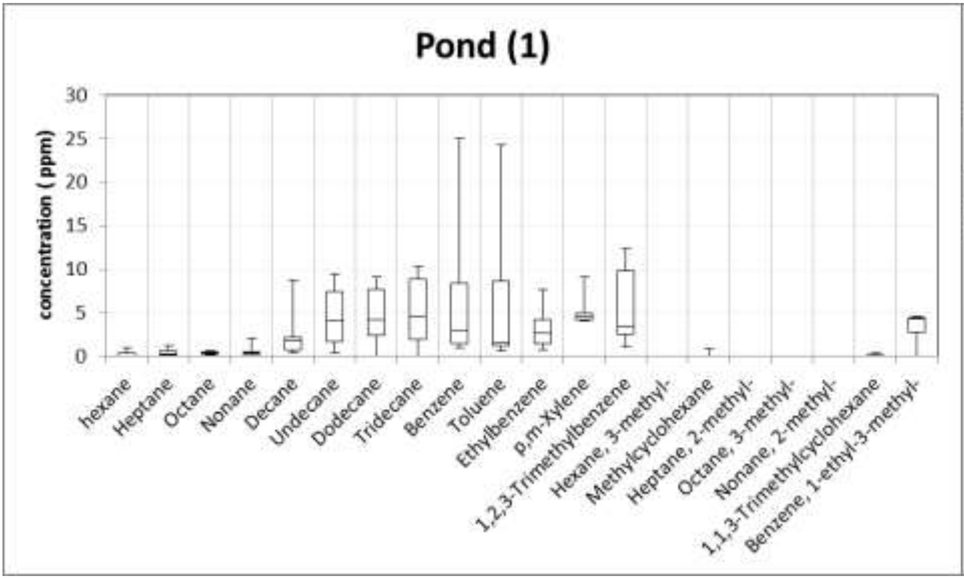
➢ Total VOCs and BTEX concentration in influent (±σ)

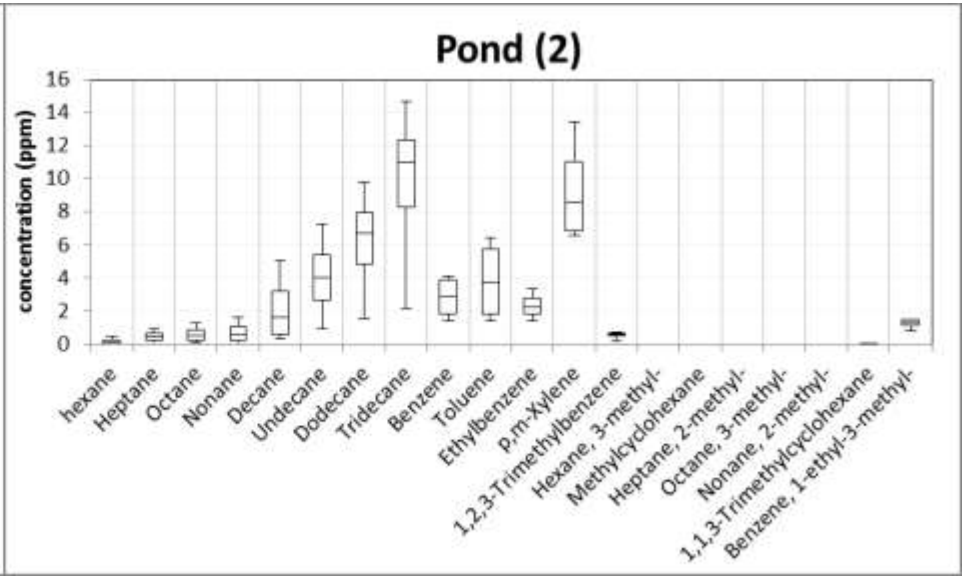


VOCs = 44±8 ppm

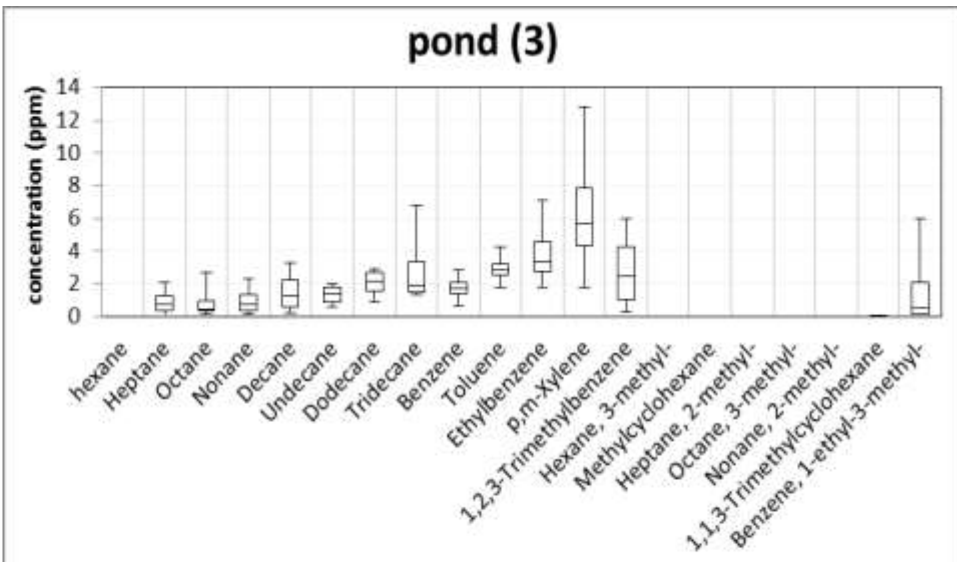
BTEX = 20±4 ppm

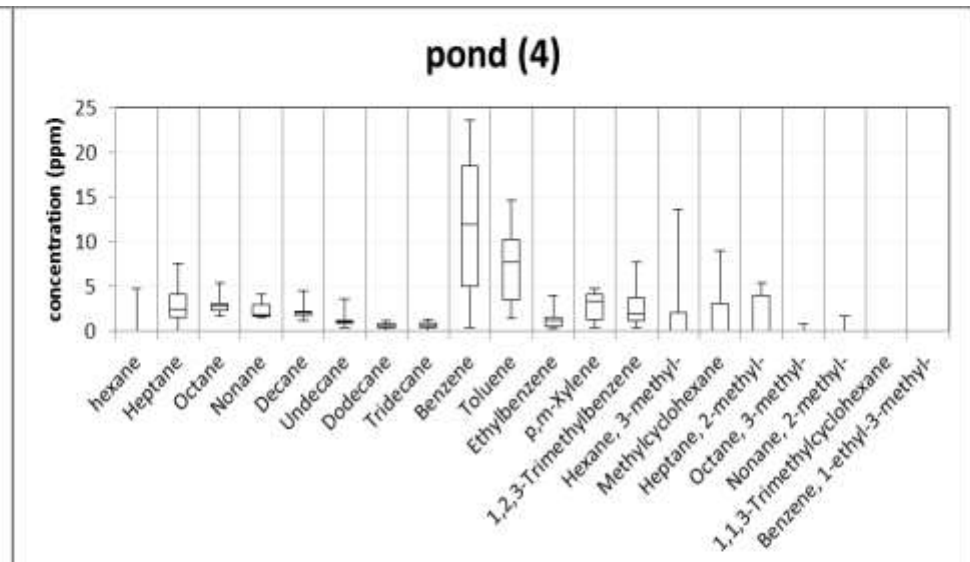
➢ VOCs speciation in influent (ppm)





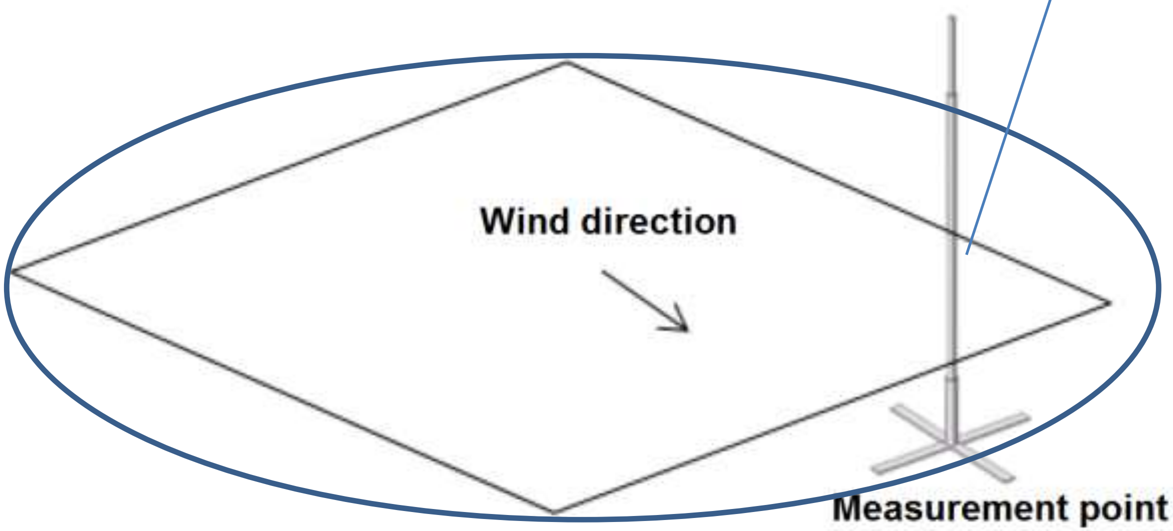
➢ VOCs concentration in influent (ppm)





VOCs measurement

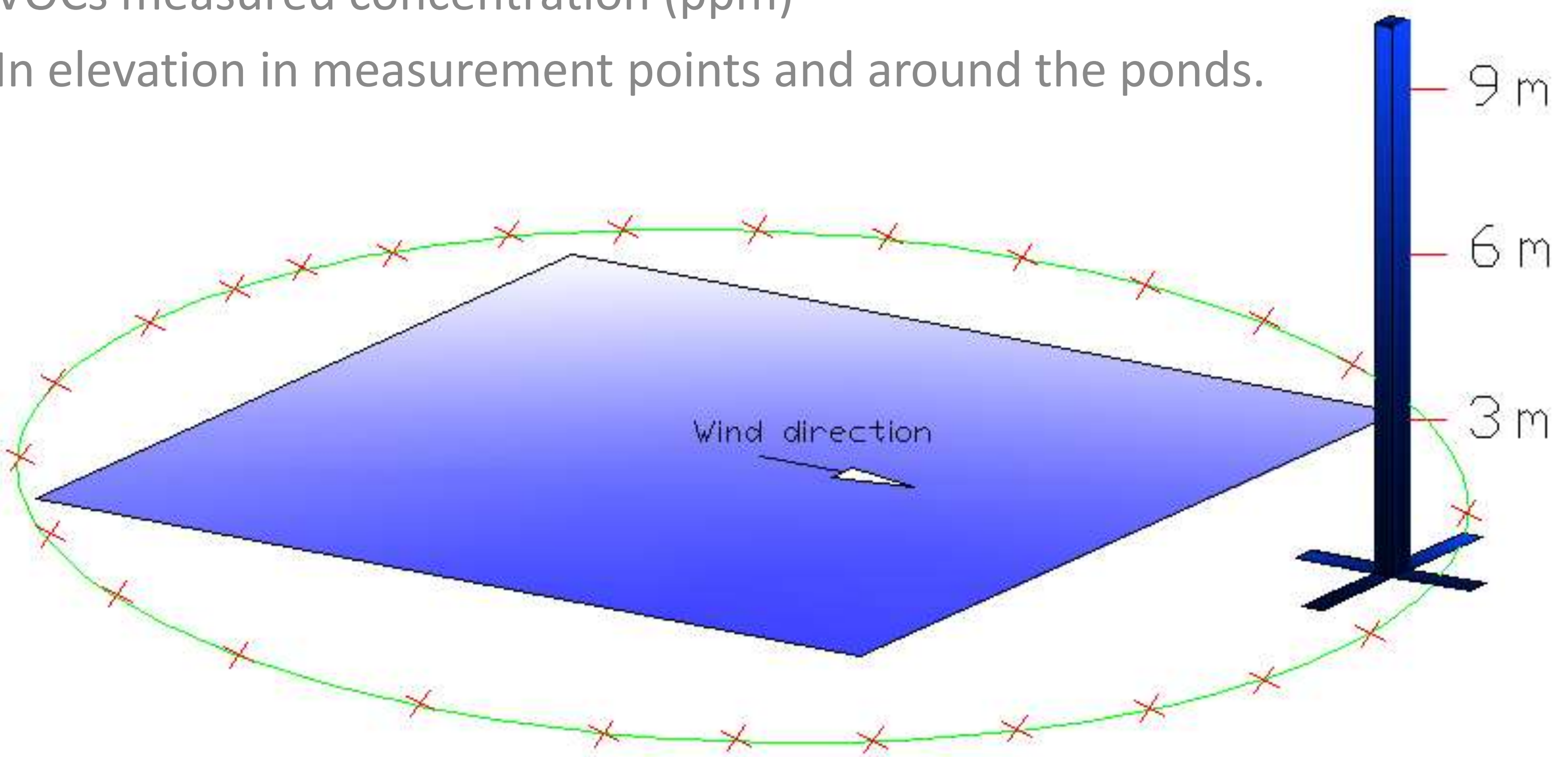
charcoal sorbent tubes



phocheck +5000

Ambient measurement points

- Around the ponds
- Height above the ground level
- VOCs measured concentration (ppm)
- In elevation in measurement points and around the ponds.



➢ Ambient measurements

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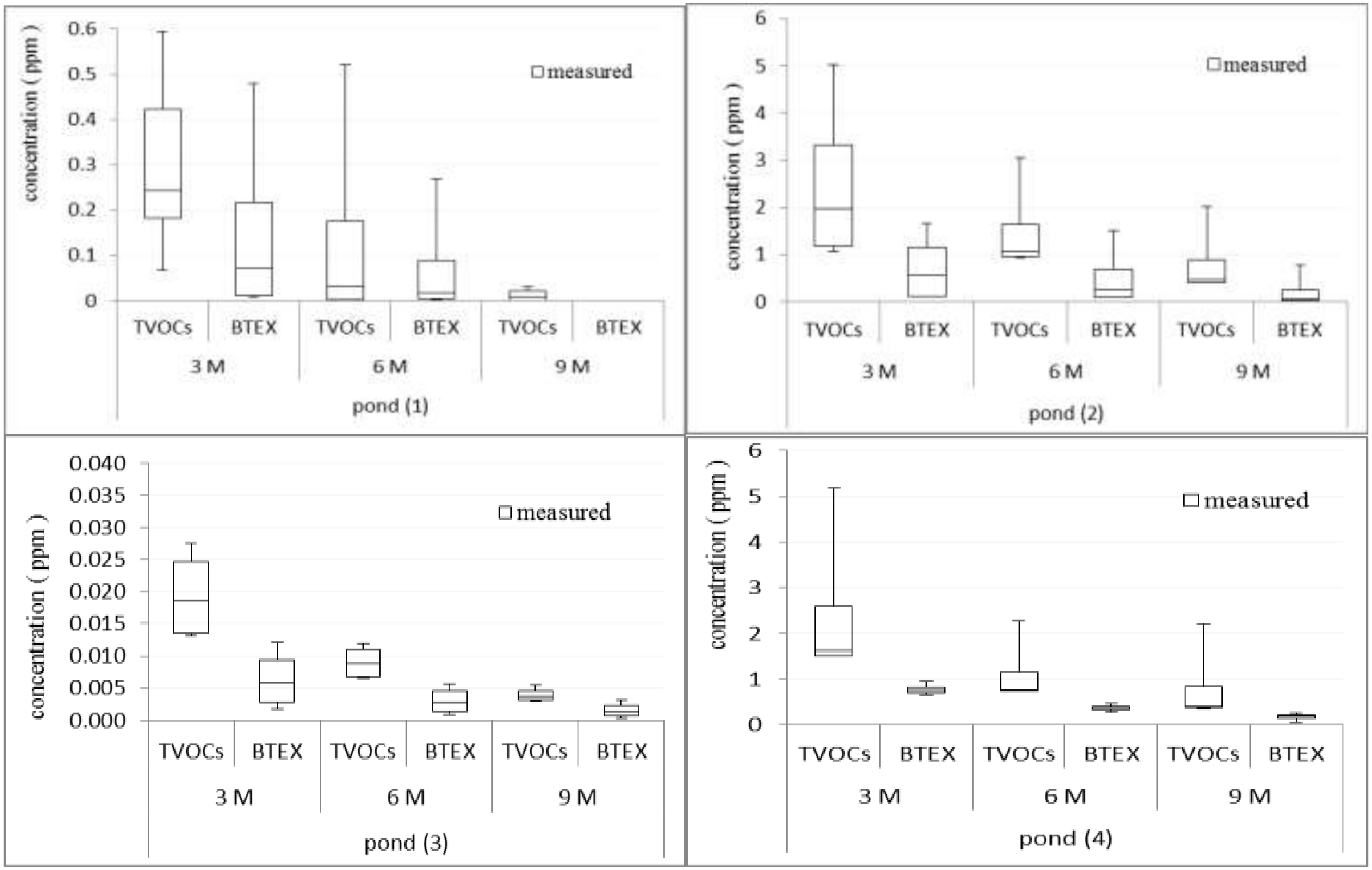
➢ Measured total VOC & BTEX in ambient

VOCs measured concentration (ppm)
At different elevations measurement points



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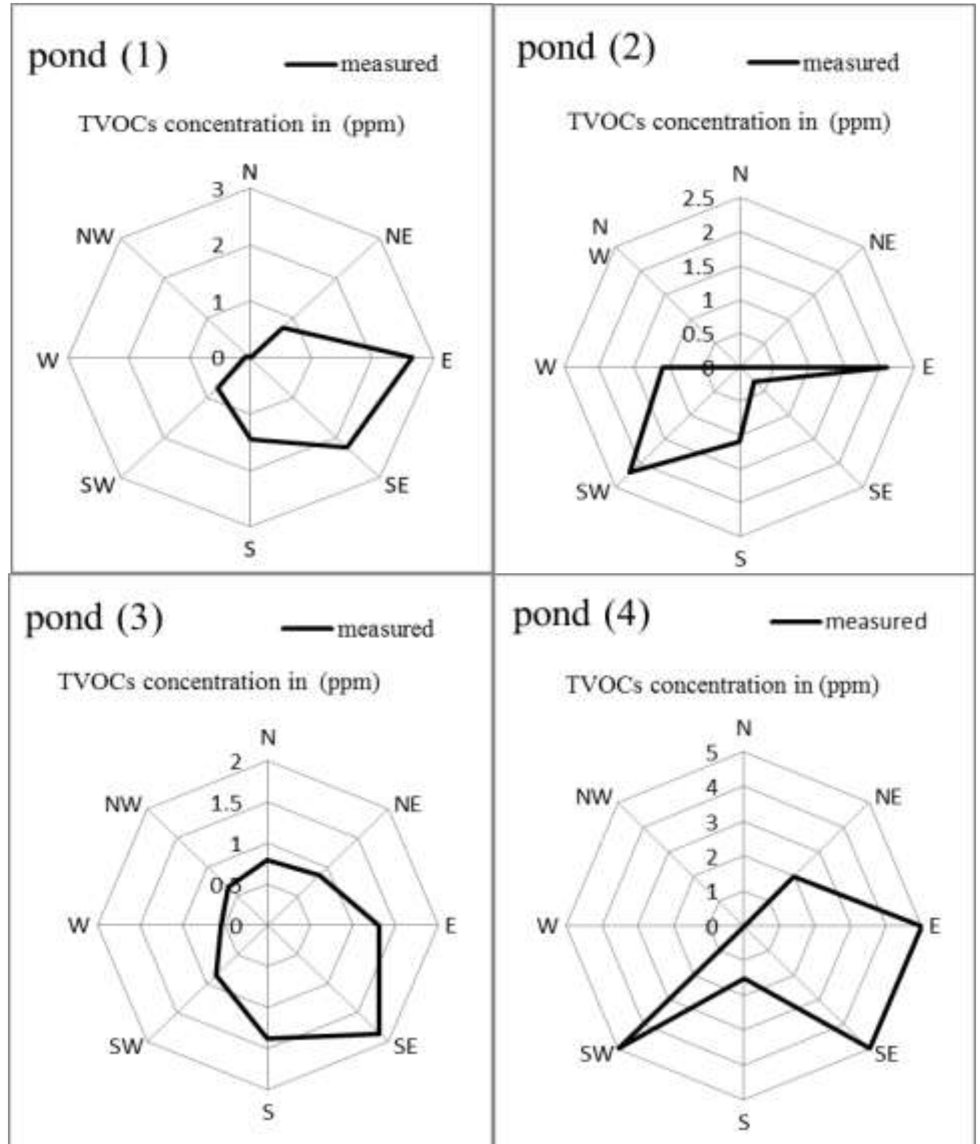
➢ Measured Ambient VOCs

(Around the ponds)

Average measured VOCs concentration around each pond



Emission Estimation (Modeling)

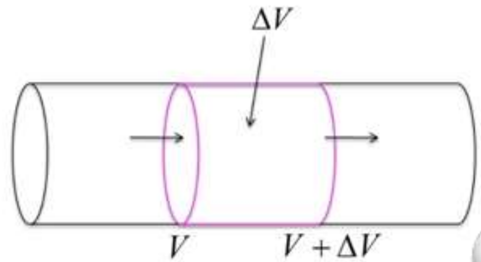
WATER9

- Wastewater collection
- Storage
- Treatment facilities
- Disposal facilities
- Evaluation of landfill
- Land treatment

- separate emission estimates for each individual compound
  - properties of the compound
  - concentration in the wastes
  - Unit operational parameter
  - meteorological parameters

➢ Emission mathematical modeling

- Reactor



$$-\frac{\delta(C_t \times V_{oil})}{\delta t} = KAC_t$$

$$t = \frac{V}{Q} \rightarrow C_t = C_l$$

$$t = 0 \rightarrow C_t = C_i$$

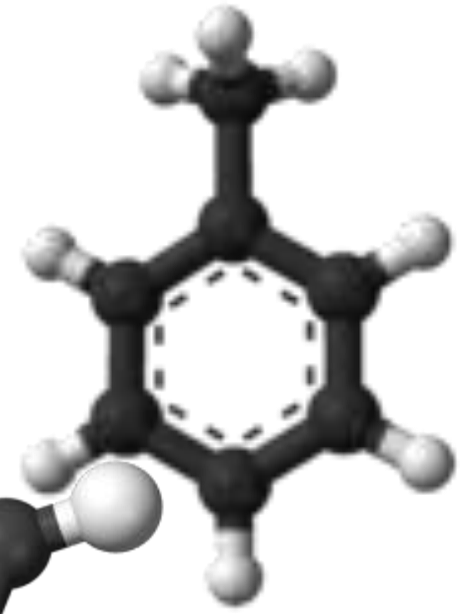
C_i = Initial component concentration
C_l = Leftover component concentration
A = Oil layer area
V_{oil} = Oil layer volume

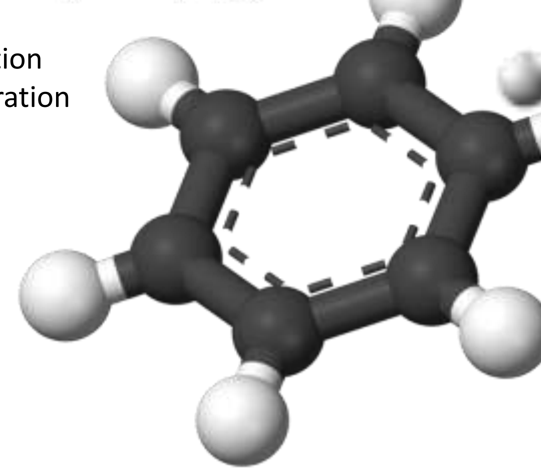
$$\left(\frac{C_l}{C_i}\right) = \mathrm{EXP}\left(-\frac{KA}{Q}\right)$$

$$(C_i - C_l) \times Q = \left(1 - \mathrm{EXP}\left(-\frac{KA}{Q}\right)\right) \times C_i \times Q$$

$$E = \left(1 - \mathrm{EXP}\left(-\frac{Kt}{D}\right)\right) \times C_i \times Q$$

t =remediation time
Q = flow rate
C_i = component concentration
D = oil layer thickness
K = overall mass transfer coefficient





overall mass transfer coefficient

$$K = k_G \times K_{eq}$$

k_G = gas-phase mass transfer coefficient

(calculated by correlation of MacKay and Mitsugu)

$$k_G = 4.82 \times 10^{-3} U^{0.78} Sc_G^{-0.67} d_e^{-0.11}$$

Sc_G = Schmidt number

d_e = Effective diameter

U = wind speed at 10 m height

K_{eq} = equilibrium constant coefficient

(Raoul's law)

$$K_{eq} = \frac{P^* \times \rho_a \times MW_{oil}}{\rho_l \times MW_a \times P_0}$$

MW_a = Air molecular weight

MW_{oil} = Oil molecular weight

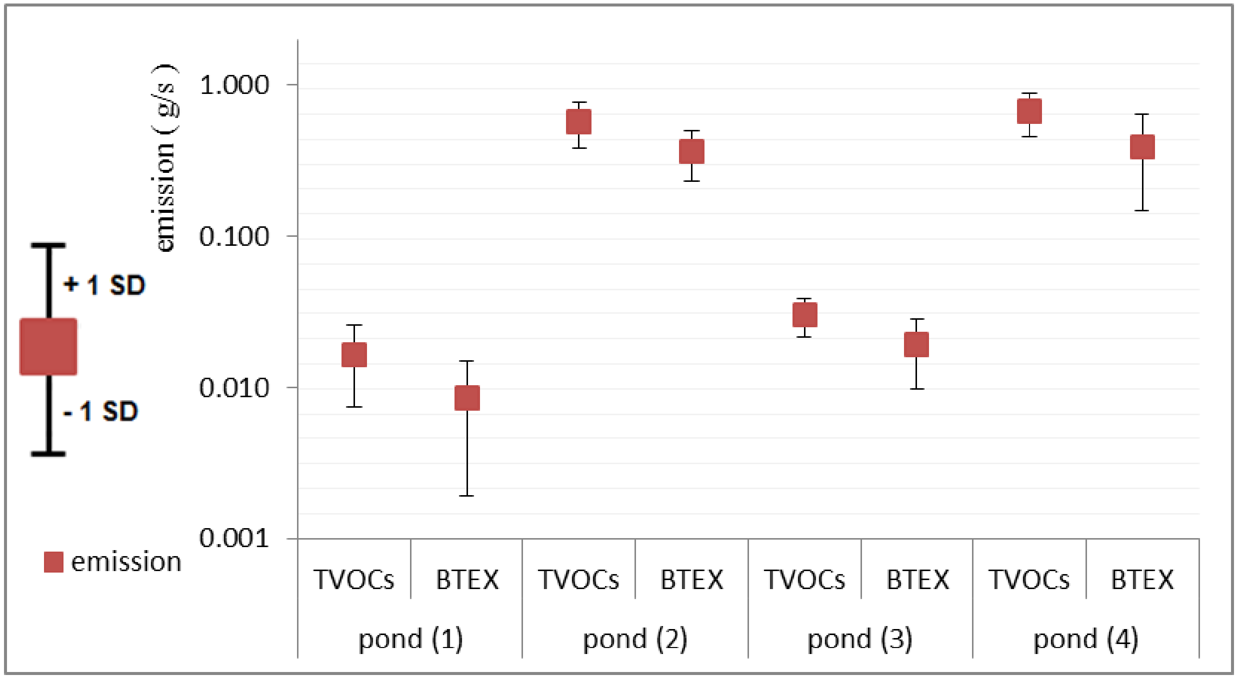
P^* = VOC Vapor pressure

ρ_l = Oil density

ρ_a = Density of air

P_0 = local atmospheric pressure

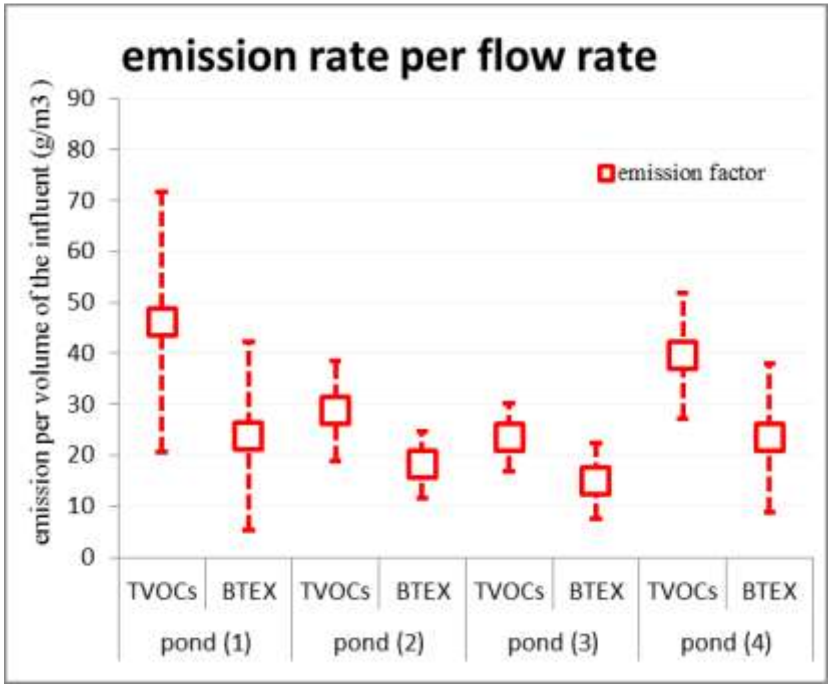
➢ Average emission rate(±σ) (g/s)



TVOCs = 0.32±0.29 g/s

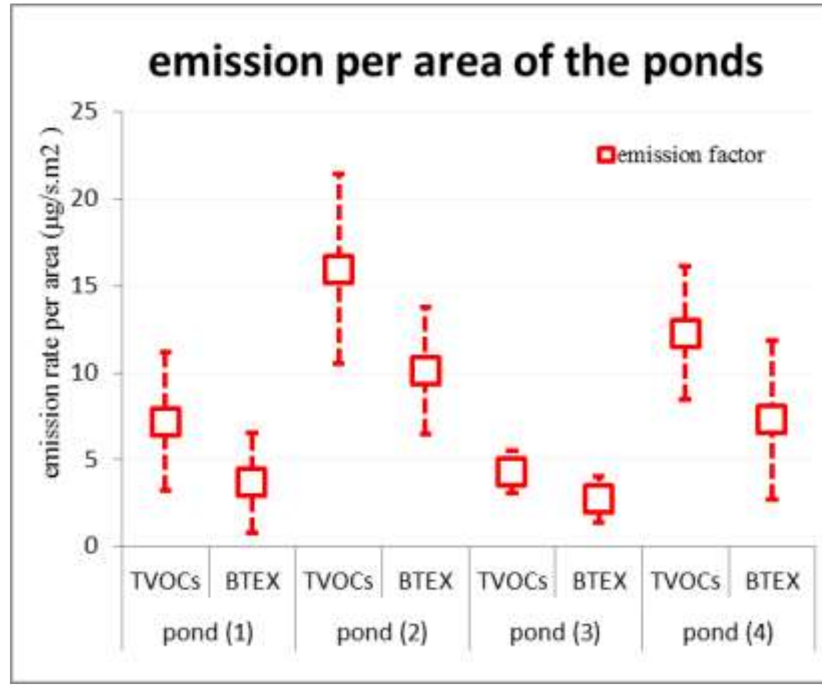
BTEX = 0.19±18 g/s

Estimate emission factor



VOCs = 34±8 g/m^3

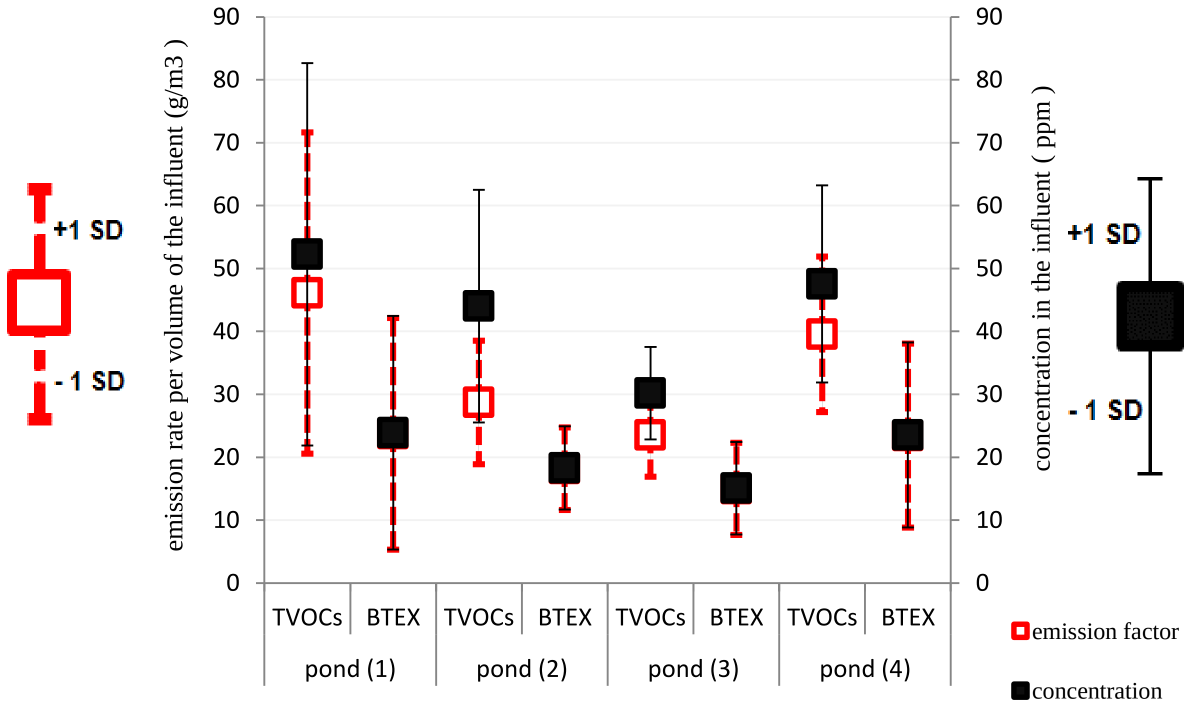
BTEX = 20±3 g/m^3



VOCs = 10±6 µg/s per m2

BTEX = 5±3 µg/s per m2

Emission percentage influent



VOCs = 80%

BTEX = 100%

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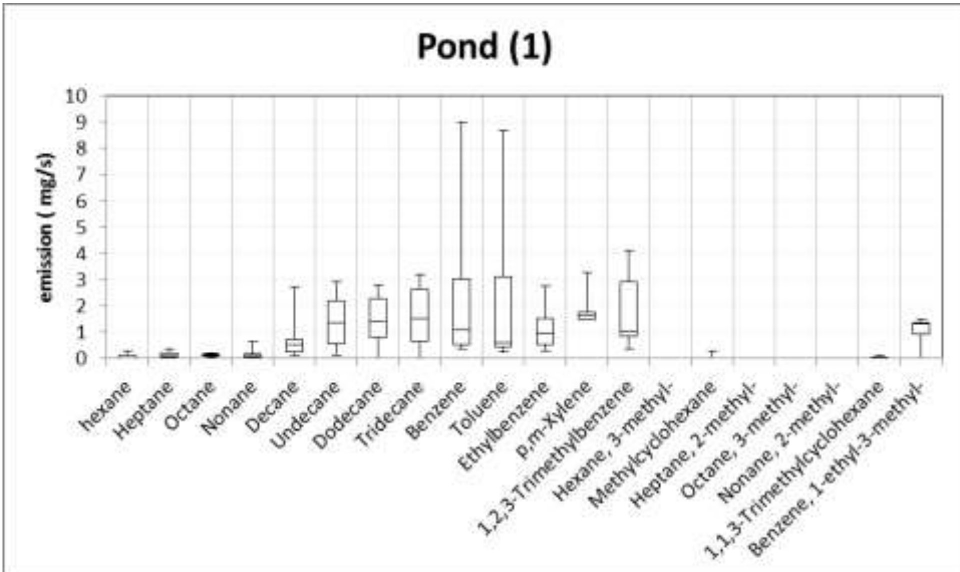
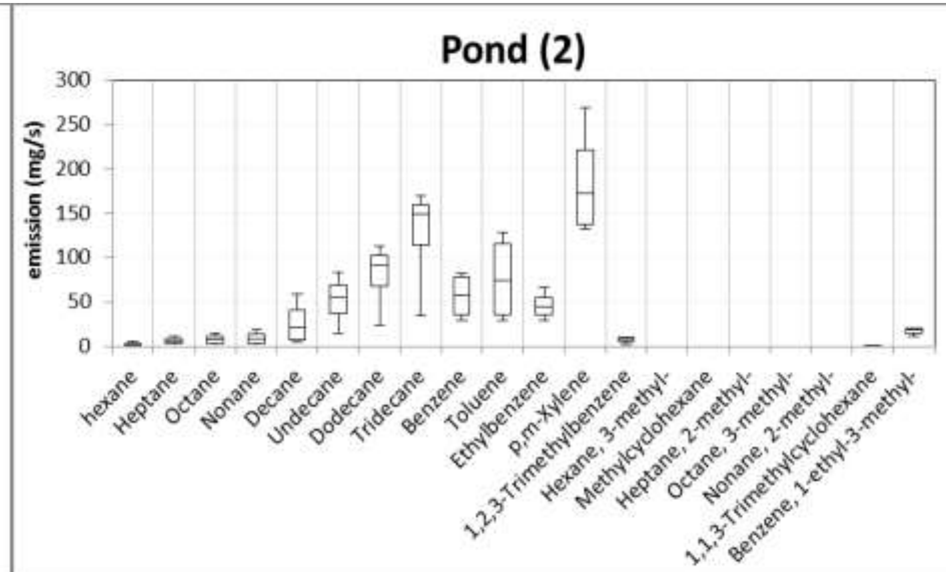
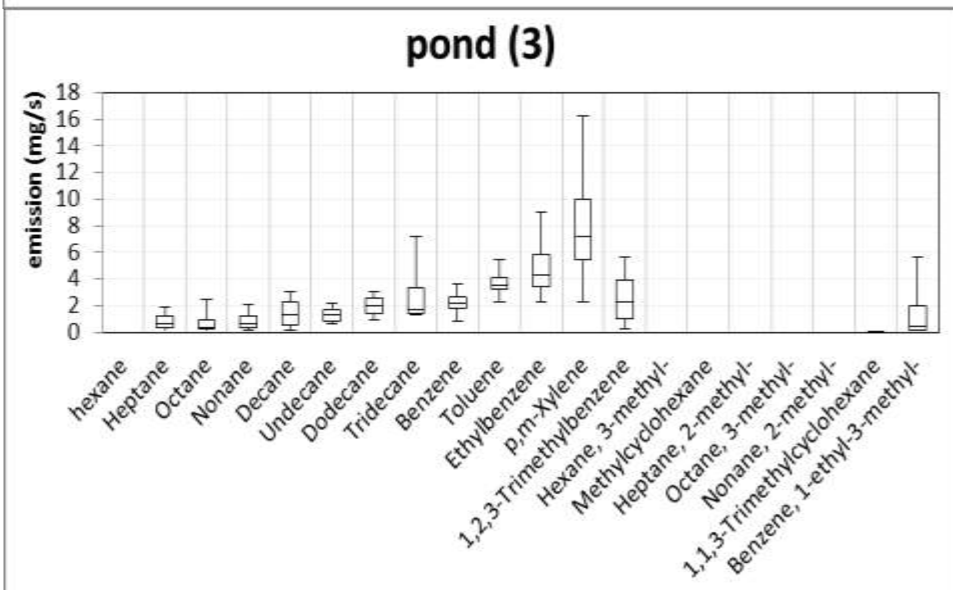
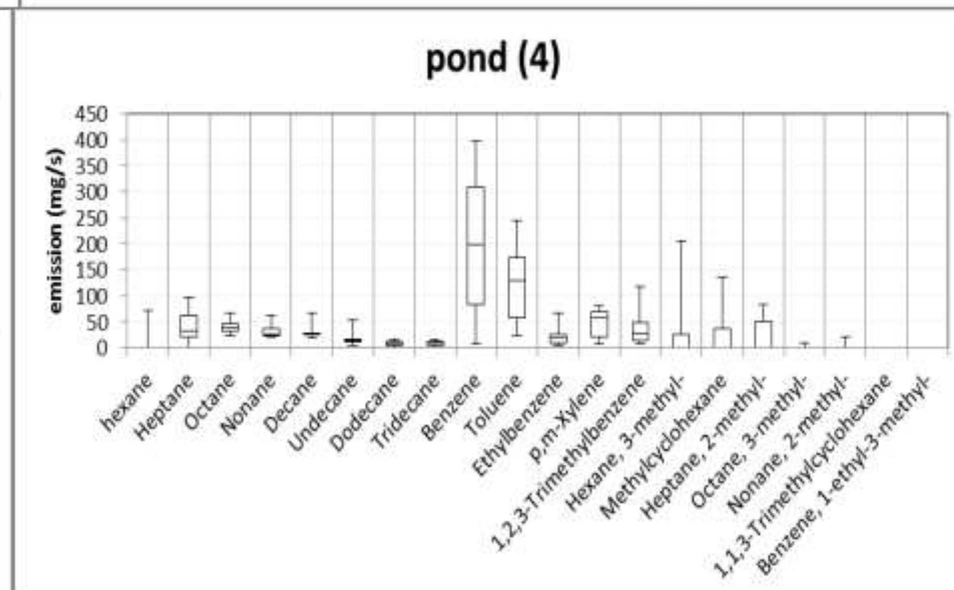
➢ Estimated VOCs emission rate (mg/s)



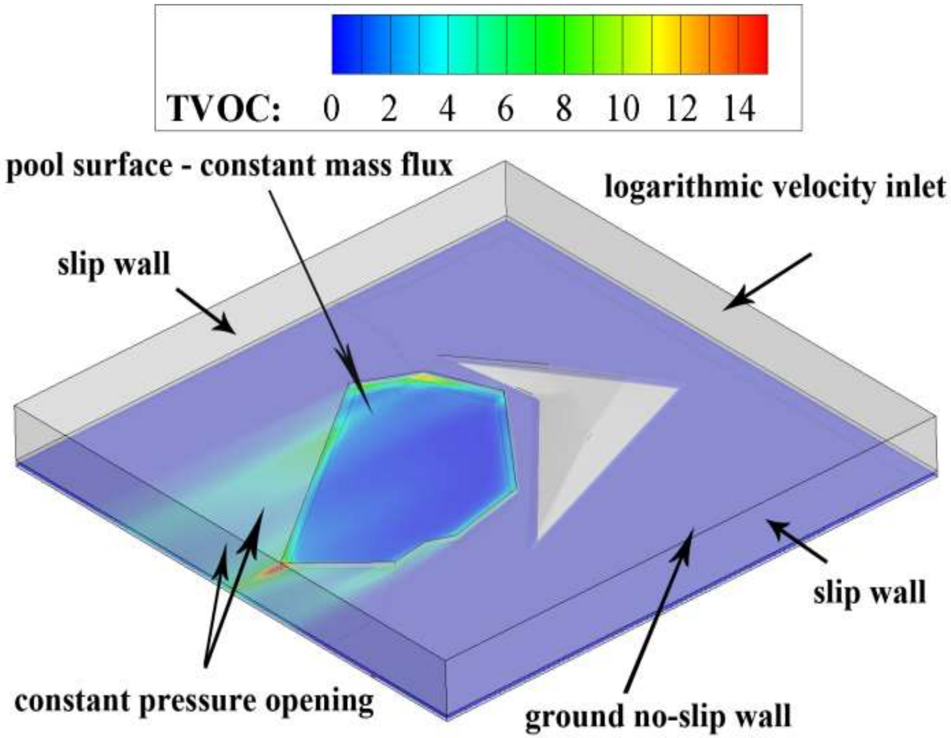






CFD simulation

- Simulate flow to obtain species field around pond
- The evaporation rate is obtained from WATER9 simulation in real condition
- Steady 3D solver
- Full size geometry
- Considering pool shape and main ground topology around the pool
- ~5M cells
- Cubic domain
- OpenFOAM® flow solver



➢ Equations

- Continuity

$$\frac{\partial \rho}{\partial t}+\frac{\partial(\rho v_i)}{\partial x_i}=S_m$$

- Navier stokes:

$$\frac{\partial(\rho v_i)}{\partial t}+\frac{\partial(\rho v_i v_j)}{\partial x_j}+\frac{\partial p}{\partial x_i}+\frac{\partial \tau_{ij}}{\partial x_j}=\rho g_i$$

- Species transport

$$\frac{\partial}{\partial t}(\rho Y_i)+\nabla\cdot(\rho\vec{v}Y_i)=-\nabla\cdot\vec{J}_i+R_i+S_i$$

- Turbulence equation: Standard k-ε

$$\frac{\partial(\rho k)}{\partial t}+\frac{\partial(\rho k u_i)}{\partial x_i}=\frac{\partial}{\partial x_j}\left[\frac{\mu_t}{\sigma_k}\frac{\partial k}{\partial x_j}\right]+2\mu_t E_{ij}E_{ij}-\rho\epsilon$$

$$\frac{\partial(\rho \epsilon)}{\partial t}+\frac{\partial(\rho \epsilon u_i)}{\partial x_i}=\frac{\partial}{\partial x_j}\left[\frac{\mu_t}{\sigma_\epsilon}\frac{\partial \epsilon}{\partial x_j}\right]+C_{1\epsilon}\frac{\epsilon}{k}2\mu_t E_{ij}E_{ij}-C_{2\epsilon}\rho\frac{\epsilon^2}{k}$$

- Spatial discretization: Finite volume

$\mathbf{j}_i^* \equiv \rho_i \mathbf{v}_i^*$ = diffusion mass flux of i species,

$X_i \equiv \frac{p_i}{p}$ = partial pressure fraction of i species,

$Y_i \equiv \frac{\rho_i}{\rho}$ = mass fraction of i species,

$p = \sum_{i=1}^{N} p_i$ = total mixture pressure,

$\rho = \sum_{i=1}^{N} \rho_i$ = total mixture density,

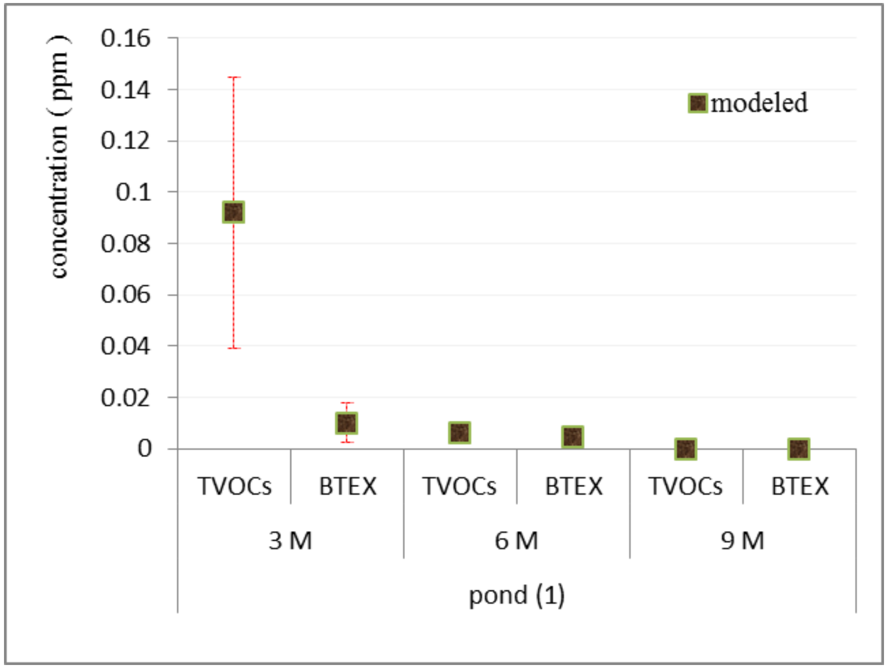
➢ CFD simulation (pond 1)

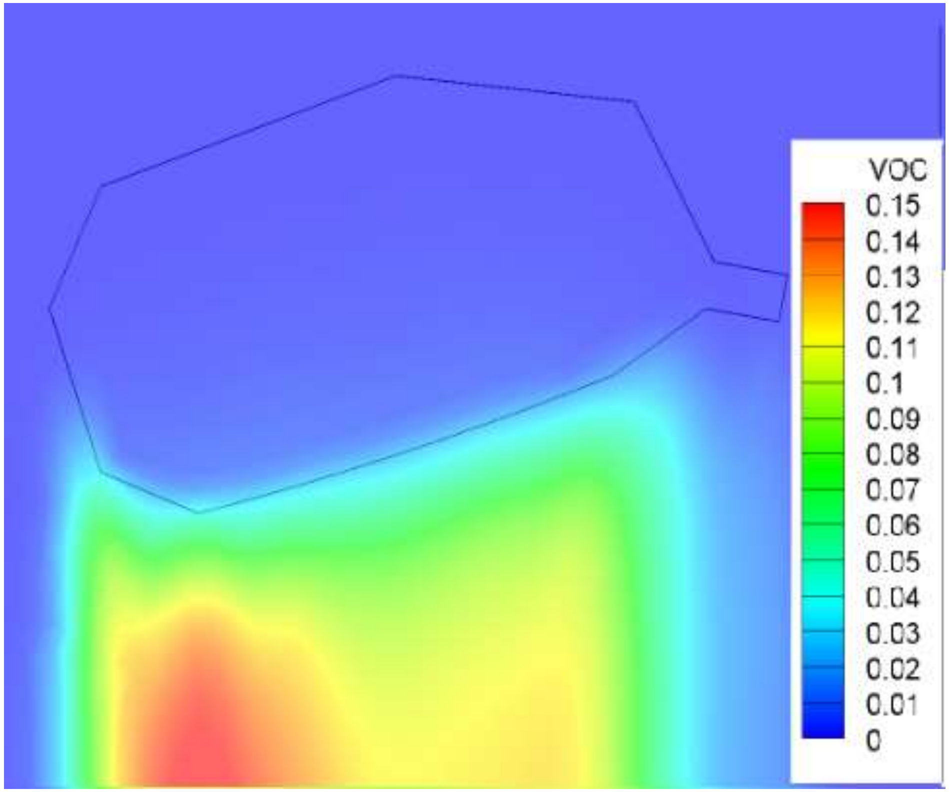
Average TVOCs emission rate:0.017±0.009 g/s

Temperature: 23-36-15-22 ˚c

Wind direction: 350-290-300-275

Wind speed: 2.7-1.5-3.0-2.1 m/s





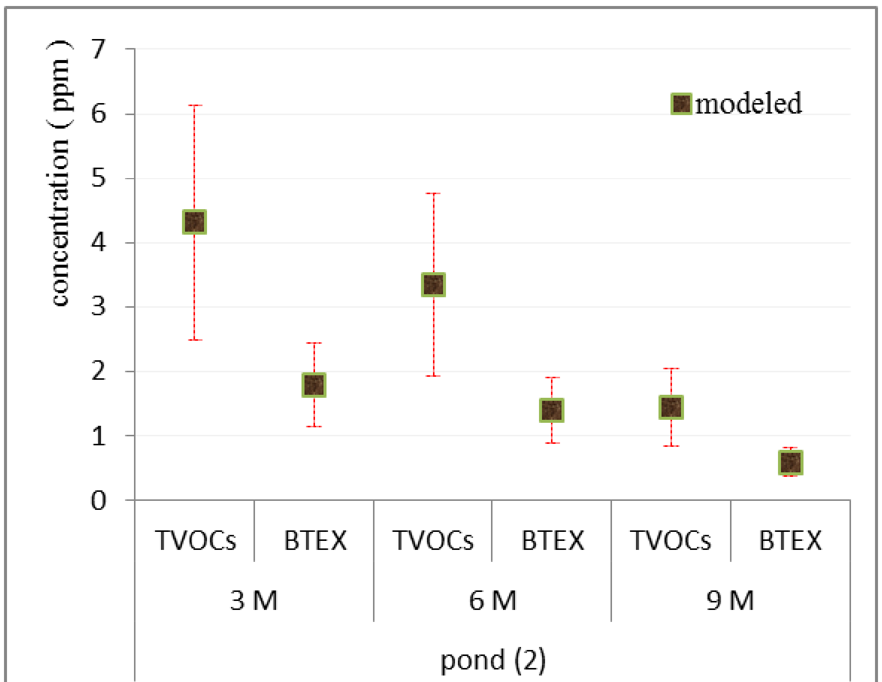
CFD simulation (pond 2)

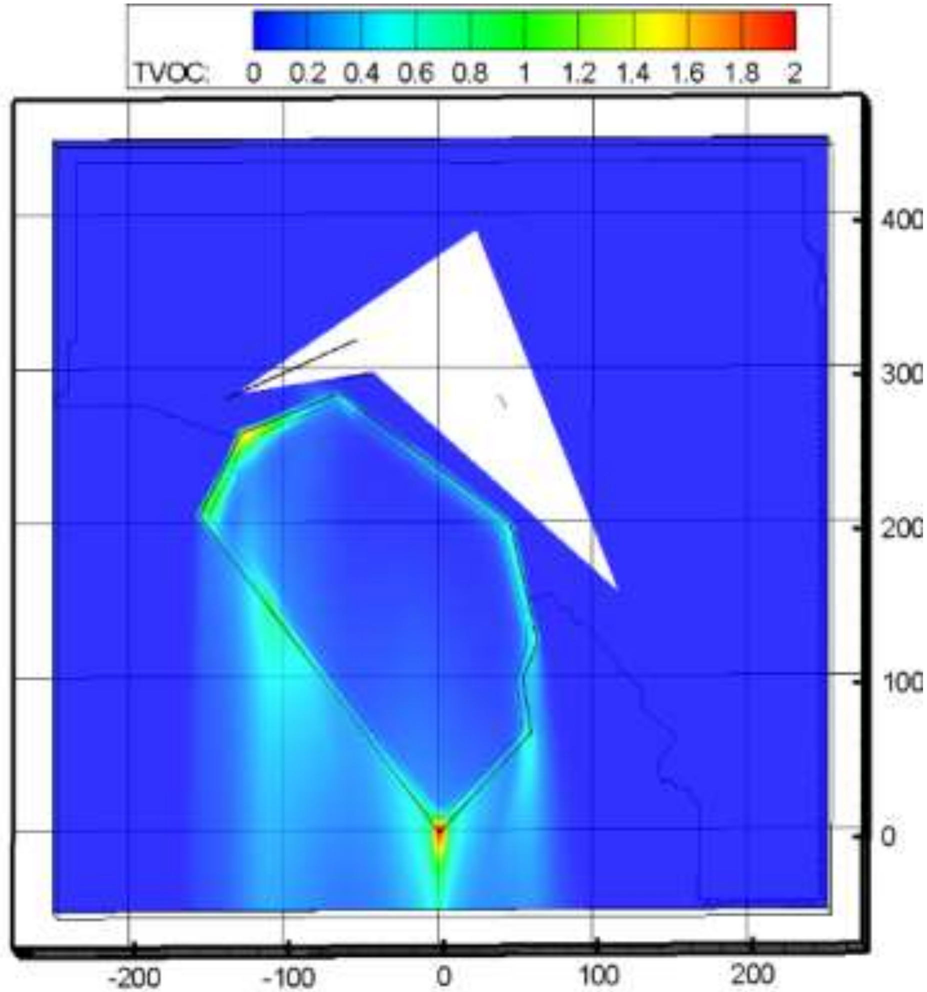
Average VOCs emission rate:0.57±0.20 g/s

Temperature: 27-16-35-21 ˚c

Wind direction: 20-310-260-360

Wind speed: 2.7-3.5-3.9-3.2 m/s





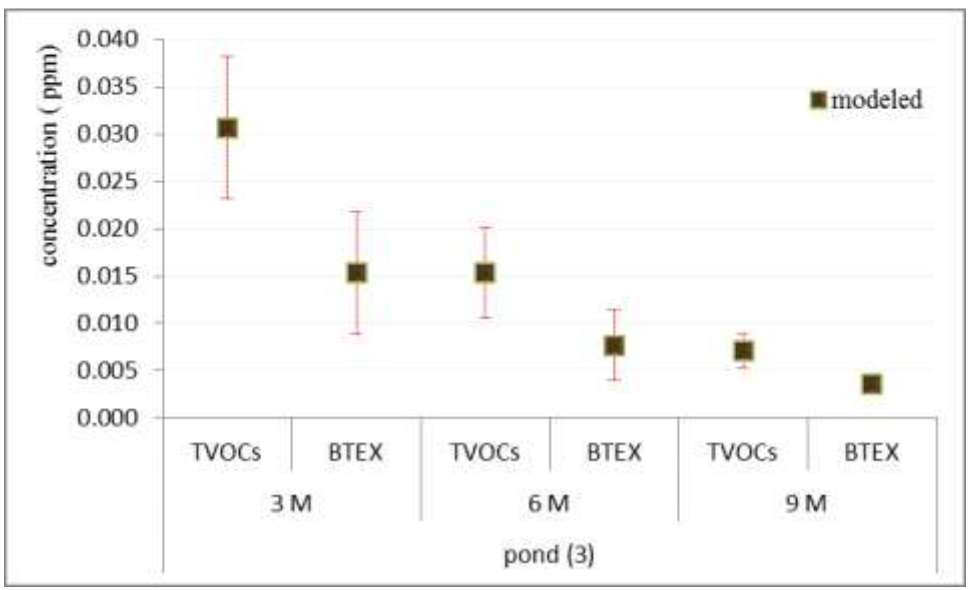
➢ CFD simulation (pond 3)

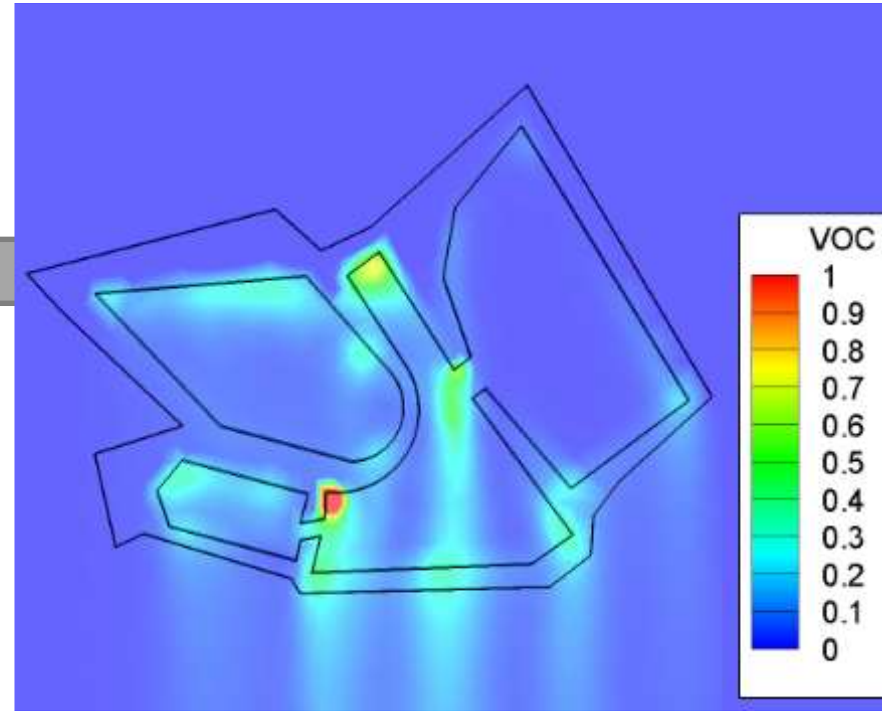
Average VOCs emission:0.030±0.008 g/s

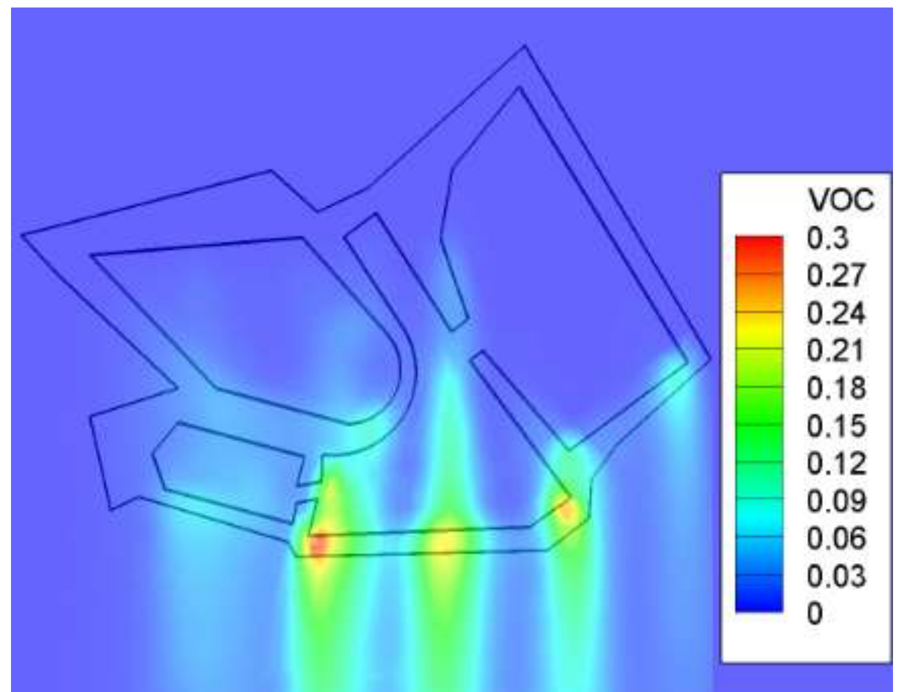
Temperature: 21-23-32-34 ˚c

Wind direction: 290-270-360-310

Wind speed: 3.5-5.4-3.5-2.1m/s







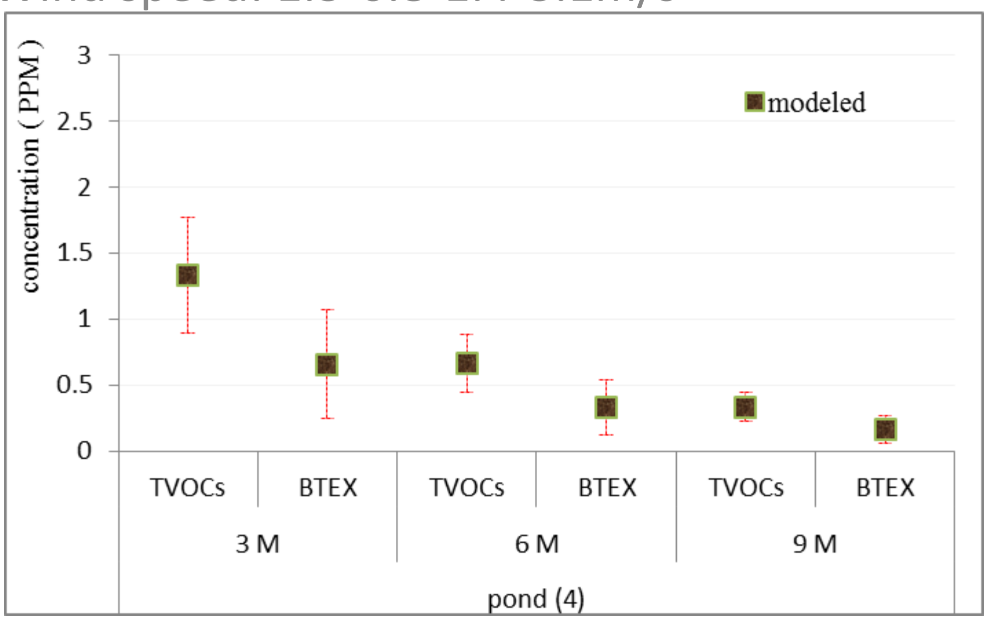
➢ CFD simulation (pond 4)

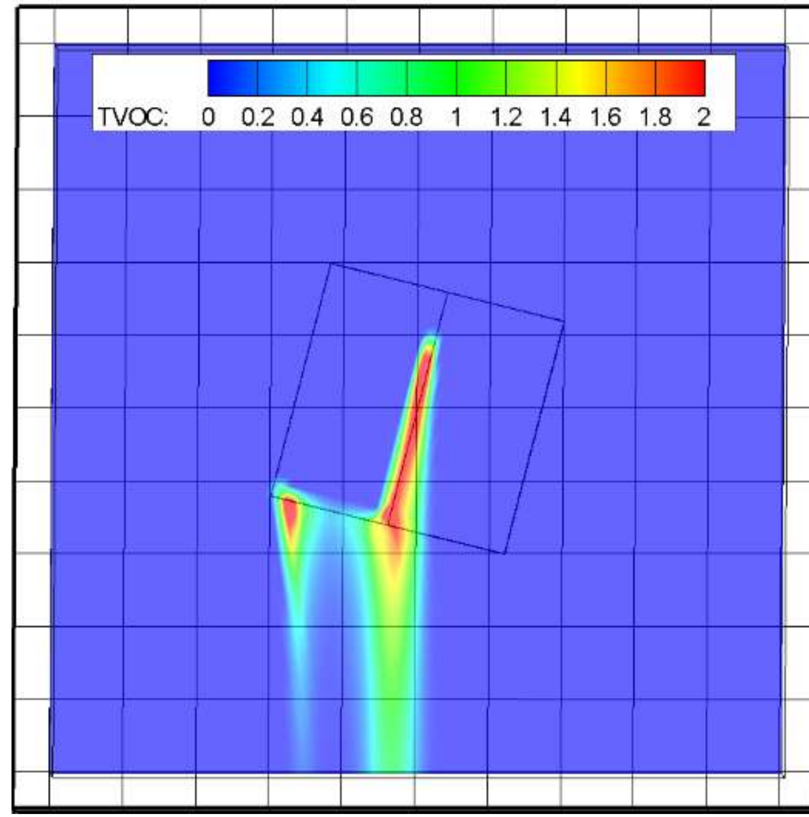
Average TVOCs emission:0.66±0.21 g/s

Temperature: 32-36-24-22 ˚c

Wind direction: 160-350-15-290

Wind speed: 1.3-0.8-1.4-3.1m/s





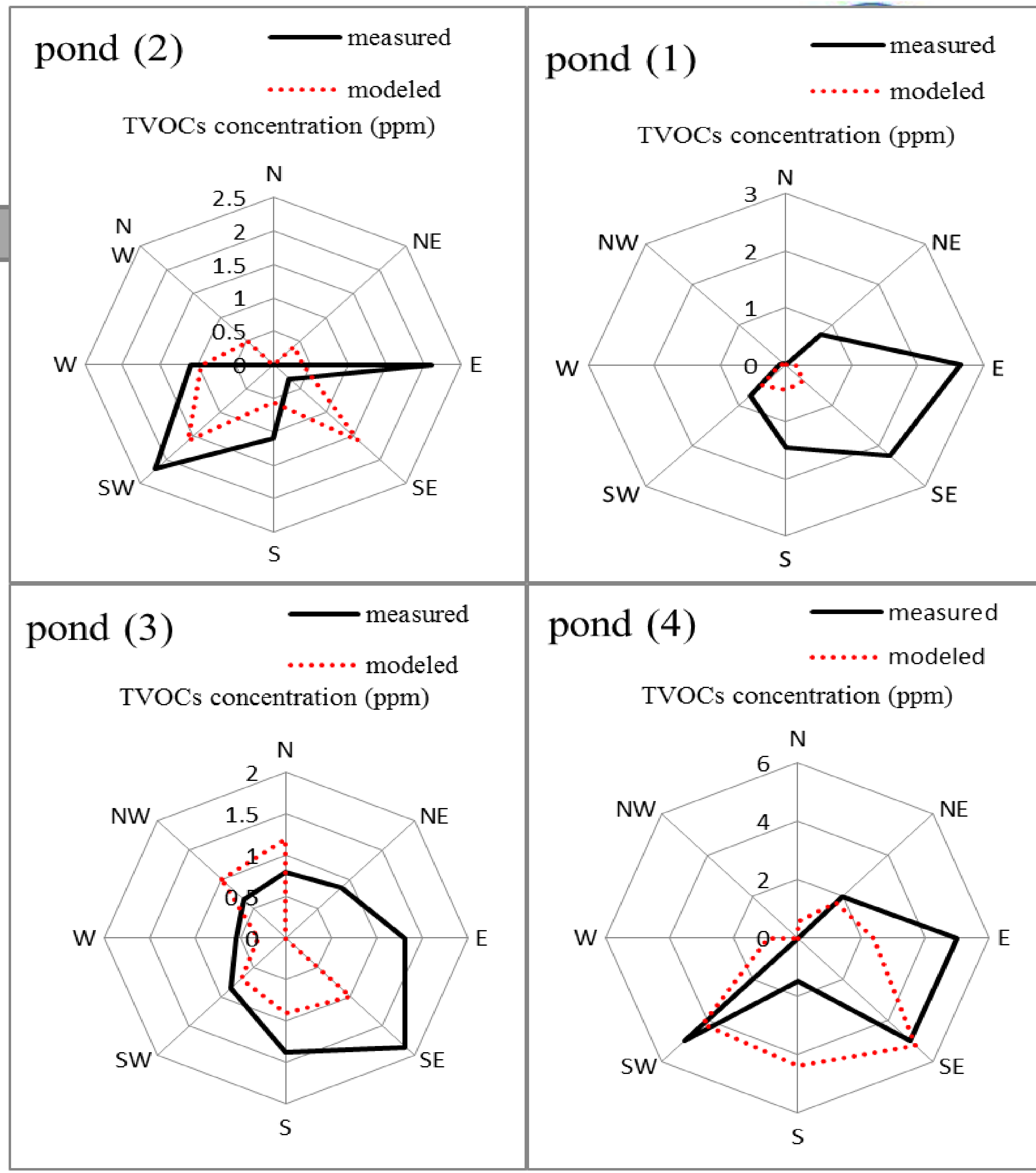
➢ Comparison

Measured VOCs

vs

Modeled VOCs

Around each ponds



➢ Modeling concentration

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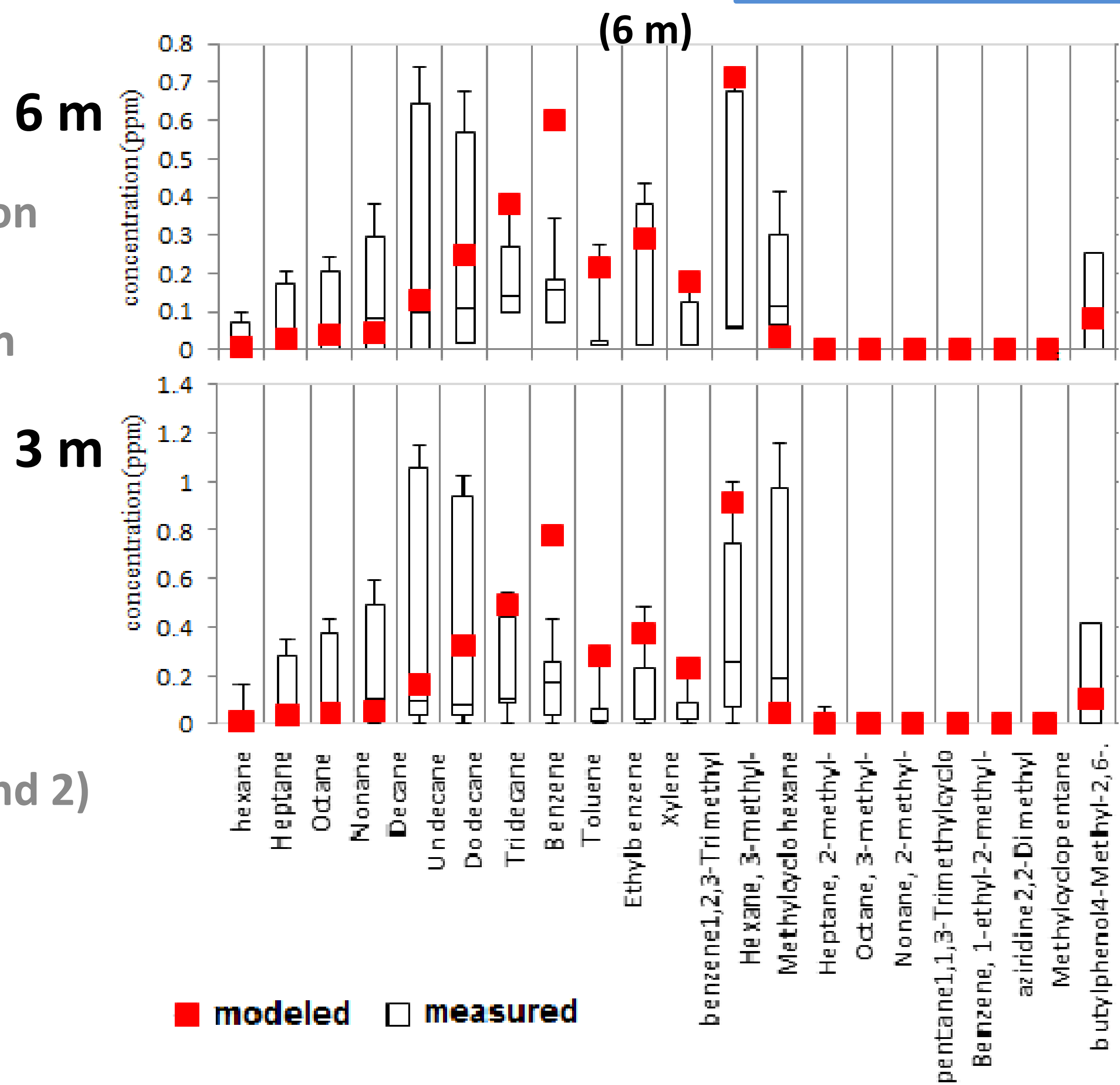
Measured VOCs concentration

vs

Modeled VOCs concentration

(VOCs in downstream of Pond 2)



➢ Modeling concentration

Measured VOCs

vs

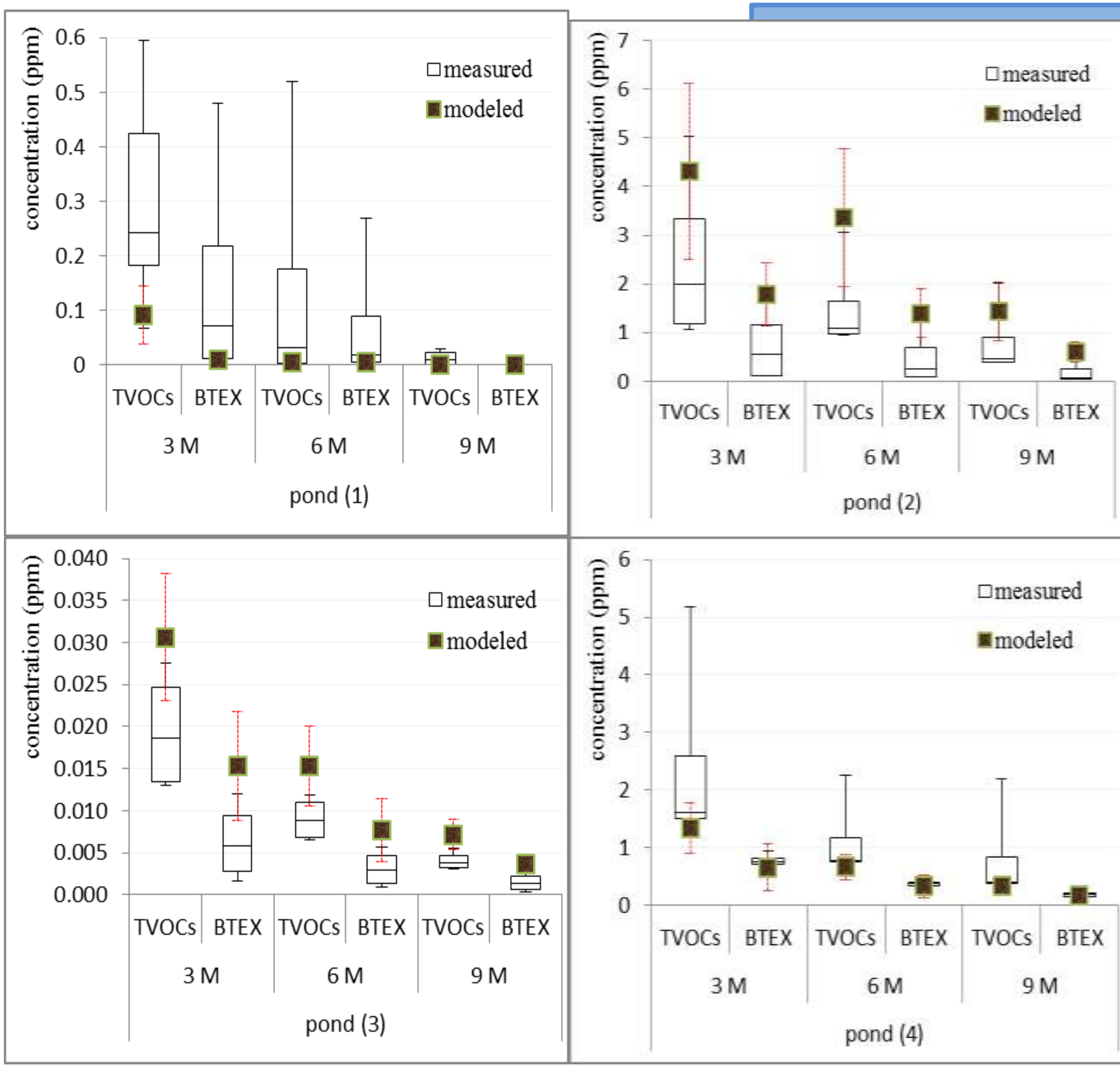
Modeled VOCs

All ponds

Different elevations

(3, 6 and 9m meters

above surface)



Conclusion

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➢ Proposed Emission Rates

	Emission (mg/s)		influence flow rate (m3/day)	Emission factor (g/m3)	
	TVOCs	BTEX		TVOCs	BYEX
Pond (1)	17 ± 9	9 ± 7	31	46 ± 26	24 ± 18
Pond (2)	574 ± 196	363 ±131	1700	29 ± 10	18 ± 7
Pond (3)	30 ± 8	19 ± 9	110	23 ± 7	15 ± 7
Pond (4)	663 ± 207	393 ± 245	1450	40 ± 12	23 ± 15
Average	**321 ± 299**	**196 ± 183**		**34 ± 8**	**20 ± 3**

$$E = Q \times F_E$$

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Thank you!

Mohammad Arhami

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