Preliminary Analysis of Self-Cleaning Capacity of Lake Pontchartrain using Fugacity Analysis

MESL RESEARCH GROUP
S. Kilic, K. Nam and M. Aral
Hurricane Katrina
A Devastated City
Short Term Solutions to Drain The City of New Orleans
Is Dilution Really the Solution?
How Long will it take Lake Pontchartrain to replenish itself?
Objective

- How long will it take Lake Pontchartrain to be “clean” again?
- The mechanisms involved
  - Dilution
  - Decay
  - Volatilization – removal by winds
  - Deposition
  - Removal with outflow
Natural Processes in the Lake

- Source
- Decay in air
  - Air particle deposition
  - Air/water absorption
  - Volatilization
- Decay in water
  - Sediment resuspension
  - Sediment deposition
  - Sediment/water diffusion
  - Sediment deposition
- Sediment
  - Decay in sediment
- Air
- Water
  - Sediment
Natural Processes in the Lake

- **In the water:**
  - Source
  - Deposition from air
  - Resuspension from sediment
  - First order decay
  - Outflow from lake

- **In the air:**
  - Volatilization from water
  - First order decay
  - Wind induced air flow out of the lake system

- **In the sediment:**
  - Deposition from water
  - Diffusion between water
  - First order decay
Mathematical Model

\[ V_w Z_{bw} \frac{dF_w}{dt} = E_w + (K_{aw} A_w Z_w + Q_{dry} Z_{aerosol} + Q_{wet} Z_{aerosol}) F_A + (Q_{res} Z_s + K_{sw} A_s Z_w) F_S \]

\[ - (k_w V_w Z_w + Q_{dep} Z_p + Q_{out} Z_{bw} + K_{aw} A_w Z_w) F_W \]

\[ V_a Z_{aw} \frac{dF_A}{dt} = (K_{aw} A_w Z_w) F_W - (Q_{dry} Z_{aerosol} + Q_{wet} Z_{aerosol} + Q_{air} Z_{ba} + K_{aw} A_w Z_w) F_A \]

\[ k_a V_a Z_a + Q_{wet} Z_{aerosol} + Q_{air} Z_{ba} + K_{aw} A_w Z_w ) F_W \]

\[ V_s Z_{bs} \frac{dF_S}{dt} = (Q_{dep} Z_p + K_{sw} A_s Z_w) F_W \]

\[ -(k_s V_s Z_s + Q_{res} Z_s + K_{sw} A_s Z_w) F_S \]
Parameters Used in the Model

- Fw : water fugacity
- Fa : air fugacity
- Fs : sediment fugacity
- Vw : volume of water
- Va : volume of air
- Vs : volume of sediment
- Aw : water surface area
- As : sediment surface area
- Qout : outgoing water flowrate
- Qair : air flowrate
- Qdep : particle deposition rate
- Qres : sediment resuspension rate
- Qdry : dry air deposition rate
- Qwet : wet air deposition rate
- t : time

- Kaw : water-air mass transfer coefficient
- Ksw : sediment-water mass transfer coefficient
- kw : water decay constant
- ka : air decay constant
- ks : sediment decay constant
- Zw : water fugacity capacity
- Za : air fugacity capacity
- Zs : sediment fugacity capacity
- Zp : water particle fugacity capacity
- Zaerosol : aerosol fugacity capacity
- Zbw : bulk water fugacity capacity
- Zba : bulk air fugacity capacity
- Zbs : bulk sediment fugacity capacity
Information Required to Solve the Governing Equations

- Information about the lake
  - Volume of lake, sediments, and air parcel
  - Surface area
  - Flow rate of outgoing tributaries
  - Air flow rate
  - Sediment deposition rate
  - Sediment resuspension rate
  - Dry deposition rate
  - Wet deposition rate
- Information about the content of the flood waters
The Contents of the Flood Waters

No information
Contaminants Selected for this Study

- **Benzene**
  - Volatile, primary pollutant, commonly used, health issues
- **Lindane**
  - Pesticide, used commonly by agricultural practice, health issues
- **PCBs**
  - Primary pollutant, recalcitrant, toxic, bioaccumulative
**Lake Pontchartrain**

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<tr>
<th>Property</th>
<th>Value</th>
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<td>Surface Area</td>
<td>1632000000 m² (630 mi²)</td>
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<td>Average Depth</td>
<td>3.65 m (12 ft)</td>
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<td>Total water outflow</td>
<td>1563352 m³/h (15336 cfs)</td>
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<td>Wind speed on lake</td>
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<td>Depth of air on lake</td>
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<td>Volume of air</td>
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<td>Depth of sediment</td>
<td>0.05 m</td>
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<td>Volume of sediment</td>
<td>81600000 m³</td>
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<td>Density of sediment</td>
<td>2400 kg/m³</td>
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Approximate scale: 30 mi (48 km)
Wind induced advection above Lake Pontchartrain

Qair = 32000000 m³/hour
Deposition and Resuspension Rates

- Adopted from a Steady-State Fugacity model development in Trent University:
  - $U_{\text{deposition}} = 0.0000005 \, \text{m/h}$
  - $U_{\text{resuspension}} = 0.0000002 \, \text{m/h}$
  - $Q_{\text{dry air deposition}} = 2.76 \, \text{m/hour}$
  - $Q_{\text{wet air deposition}} = 7.34 \, \text{m/hour}$

(http://www.trentu.ca/cemc/models)
Mass Transfer Coefficients

- Two-film theory to calculate for each contaminant
- Overall water-air mass transfer coefficient:

\[
\frac{1}{K_{aw}} = \frac{1}{k_{water}} + \frac{1}{k_{air} H}
\]

- \( K_{aw} = 0.0034 \text{ m/hour for PCBs} \)
- \( K_{aw} = 0.00002 \text{ m/hour for Lindane} \)
- \( K_{aw} = 0.00958 \text{ m/hour for Benzene} \)
Physicochemical Properties Required for Contaminants

- Water Solubility
- Vapor Pressure
- Octanol-Water Partition Coefficient
- Density
- Molecular Weight
- Half lives in each media

\[
Z_{air} = \frac{1}{RT}
\]

\[
Z_{water} = \frac{1}{H} = \frac{C^s}{P_s}
\]

\[
Z_{sediment} = \frac{K_{sw} \rho_s}{H} = K_{sw} \rho_s (Z_{water})
\]

\[
k_{reaction} = \frac{Ln2}{\tau_{1/2}}
\]
Source Rate

- The pumping lasted about one week
- About 10% of lake volume was pumped into the lake
- 3420000 m³/hour source rate
- 10 % of the dumped water is contaminant by volume.
- Convert to mass rate for each contaminant
  - 2200000000 moles/hour Lindane
  - 3840000000 moles/hour Benzene
  - 14700000000 moles/hour PCB
Solution Technique of the System of Equations

- The nonlinear model yields three equations with three unknowns.
- Finite Difference Method is used to solve the governing equations.
- A matrix solution algorithm is developed for simultaneous solution.
## Final Values Used in the Model

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<th>BENZENE</th>
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Results

- It will take Lake Pontchartrain:
  - 1 year to recover from Benzene pollution.
  - 13.5 years to recover from Lindane pollution.
  - 81 years to recover from PCB pollution.

- Regulated standard values by EPA in water:
  - Benzene 0.005 mg/L.
  - Lindane 0.0002 mg/L.
  - Total PCBs 0.0005 mg/L.
PCB Results

Aqueous PCB Concentration in Lake Pontchartrain

Air PCB Concentration above Lake Pontchartrain
How Lake Pontchartrain Reacts to Contaminant Dumping Water

Aqueous PCB Concentration in Lake Pontchartrain

When water pumping stops
PCB Results

Sediment PCB Concentration in Lake Pontchartrain

- Concentration (mg/L)
- Time (days)

- Concentration (mg/L)
- Time (years)
PCB Results

Aqueous PCB Concentration
years 12 - 37
Lindane Results

Aqueous Lindane Concentration in Lake Pontchartrain

Air Lindane Concentration above Lake Pontchartrain
Lindane Results
Benzene Results

Benzene Concentration in Lake Pontchartrain

Aqueous Benzene Concentration in Lake Pontchartrain
Benzene Results

Air Benzene Concentration above Lake Pontchartrain

Sediment Benzene Concentration in Lake Pontchartrain
Some Observations

- Air Phase recover quickest for all three contaminants
- As Benzene is more volatile, it partitions into air sooner and removed from the system – about 1 year
- PCB stays longest – 81 years
- All three chemicals stay longest in the sediments
- Benzene partitions more proportionally among three phases
## Sensitivity Analysis - PCB

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## Sensitivity Analysis - Benzene

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</tr>
</tbody>
</table>
Observations about Sensitivity Analysis (1)

- The most important parameter is sediment reaction rate constant (ks) – derived from half lives
- The higher the half life in sediment, longer it takes the lake to recover
- The second most effective parameter is sediment-water mass transfer rate (Ksw). When the contaminant passes to sediment, it takes it longer to get out of the system.
- On the other hand, air-water mass transfer rate (Kaw) has the inverse effect. As the contaminant passes into air, it is removed from the system quicker, due to faster decay and air outflow
Observations about Sensitivity Analysis (2)

- Benzene is more sensitive for parameter changes.
- Benzene is more volatile, thus when air-water mass transfer coefficient is higher, removal of benzene from the system is quicker.
Conclusion

- **Hydrophobicity.** Higher the octanol-water partition coefficient, longer it will take a lake to replenish (PCB – 6.6; Benzene – 2.13; Lindane – 3.70)
- **Volatile compounds will be removed faster,** however will create air pollution problems in the immediate vicinity.
- **During the first couple of weeks following the dumping of the flood waters,** some living organisms must have been harmed as the contaminants reach very high concentrations in the lake.
Ongoing Work:

- Inclusion of bioaccumulation module to this model.
- Consider speciation.
- Develop a dynamic model, which also has a spatial variability.
- Uncertainty analysis.
For additional information or questions, you may contact:

M. M. Aral: maral@ce.gatech.edu

Or visit MESL web page at

http://www.ce.gatech.edu/research/MESL/