Coupling of Water and Atmosphere Reactive Transport Simulations - the New 3D SMART Model

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Table of Content

• Concept of Coupled Sea-Atmosphere Simulations
• Boundary Conditions
• Meshing
• FLUENT Simulation for the Atmosphere
• Demonstrator for Coupled Sea-Atmosphere Simulation
• Conclusions & Prerequisites
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Hydrodynamic Coastal Model (E.g. FVCOM)

Coastal Unstructured Meshing (E.g. SMS)

Hydrodynamic fields

Seawater Biocide Model
(Providing kinetic rates for decay & halogenated byproduct formation;)

Water & Air Quality Model
1. Preprocess sub-mesh & water quality boundary conditions
2. Species fate simulation
3. Visualization

Atmospheric Model (E.g. FLUENT)

Marine Life Model
(Oxidants and halogenated organic matter toxicity & species decay)
## Boundary Conditions

<table>
<thead>
<tr>
<th>Boundary Condition with $\mathbf{n} \perp \partial \Omega$</th>
<th>FVE-approximation $\forall , ihk$ corresponding to the BC</th>
</tr>
</thead>
<tbody>
<tr>
<td>Horizontal Open [ 0 = \frac{\partial c}{\partial n} \bigg</td>
<td>_{n=0} ]</td>
</tr>
<tr>
<td>No-flux [ 0 = \mathbf{u}c - D \frac{\partial c}{\partial n} \bigg</td>
<td>_{n=0} ]</td>
</tr>
<tr>
<td>Sea Boundary Layer [ c_w = \frac{c_{at}}{k_{eq}} \land \frac{\partial c}{\partial z} \bigg</td>
<td>_{at , intf} = 0 ]</td>
</tr>
<tr>
<td>Air Boundary Layer [ c_w = \frac{c_{at}}{k_{eq}} \land \frac{\partial c}{\partial z} \bigg</td>
<td>_{at , intf} = 0 ]</td>
</tr>
<tr>
<td>Sea Boundary Layer with constituent in atmosphere [ c_w = \frac{c_{at}}{k_{eq}} \land \frac{\partial c}{\partial z} \bigg</td>
<td>_{at , intf} = 0 ]</td>
</tr>
<tr>
<td>Vertical air BC at atmospheric top-layer [ D \frac{\partial c}{\partial z} \bigg</td>
<td>_{z=0^-} = D \frac{\partial c}{\partial z} \bigg</td>
</tr>
</tbody>
</table>
Coupling of Water and Atmosphere Reactive Transport Simulations - the New 3D SMART Model
- Horizontally unstructured triangle mesh
- Surface elevations
- Sub-layer
- Atmosphere
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A: Average of upper atmosphere layer.
B: Lower two atmosphere layer.
C: Top-layer sea.
D: Average sea except top layer.
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Precursor Simulations

Joint sea and atmosphere species transport precursor simulations are carried out as byproduct of existing projects:

- Arabian Gulf model
Conclusion

The 3D SMART is capable to simulate coupled sea-atmosphere natural gas plumes.

Identified Prerequisites

• Calibrated Arabian Gulf model including all data (bathymetry, salinity fields, tidal data etc.)
• 3 models coupled and ran on the same super computer
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