

Supplemental Information for: *Emissions of Organic Compounds from Produced Water Ponds II: Emissions of Organic Compounds from Produced Water Ponds II: Evaluation of flux-chamber measurements with inverse-modeling techniques*

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OpenFOAM Analyses

We used OpenFOAM v.4.1 with HELYX-OS (<http://engys.com/products/helyx-os>) as Graphical User Interface to simulate wind field at the produced water pond discussed in Case Study. We simulated the pond as a simple 3-dimensional cavity constructed by a mesh of 0.1 m hexahedral cells. The pond cavity has area of 0.27 ha at the bottom that represents the water surface, and 0.32 ha at the top that represents the ground-level area enclosed by the berms (Figure S1). We simulated the water surface as a slip wall, the surrounding berm interfaces as four 1:2 slope no-slip fixed walls, and the top plane as a moving wall that moves at the wind speed of 2.4 m s⁻¹ measured at 6 m above ground level. We simulated wind over the pond as steady-state incompressible flow and specified enough run time to obtain results at steady state. Finally, we performed sensitivity simulation with several choices of low-Reynolds turbulence model that are available in OpenFOAM but found insignificant differences in the results.

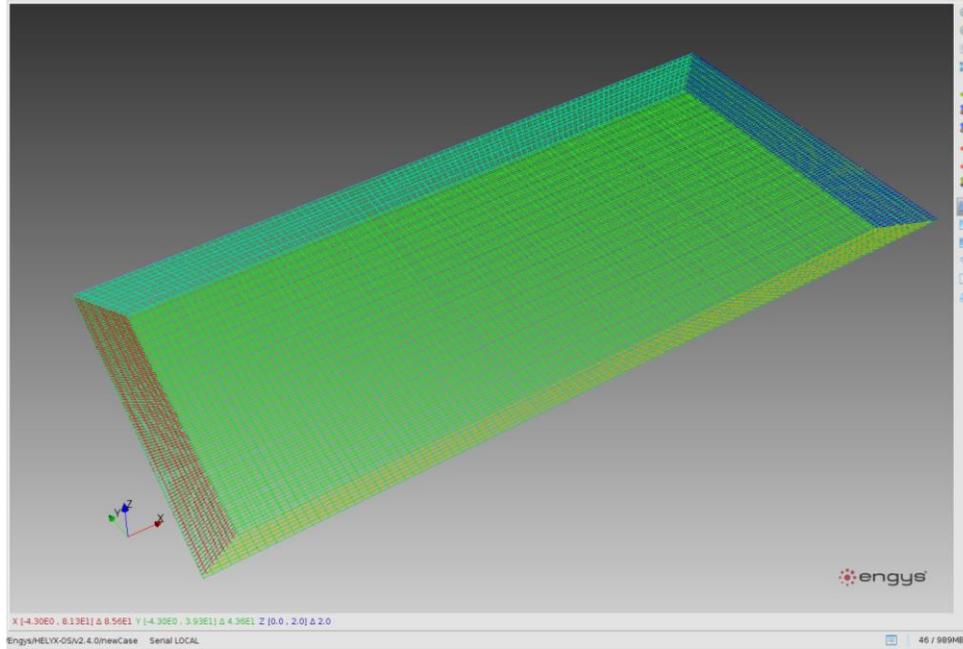


Figure S1. OpenFOAM 3-dimensional mesh configuration of the produced water pond in Case Study. The origin is set at the north corner of the pond. We set the top wall to move in from bottom-left to upper-right direction and at 43 degree from the x-axis to replicate the north-north-east wind in the Case Study.

Figure S2 shows wind vectors at water level at steady state. Two significant findings: firstly, wind speeds at water level are about 0.5 m s^{-1} in comparison with 2.4 m s^{-1} input wind speed at 6 m above ground level; secondly, wind takes up emissions from the lower end of the pond (east side of the pond as in Figure S2) and transports it to the upper end of the pond, where it swirls and exits from the upper end. The implication is that emissions from the lower end of the pond do not directly reach receptors in that area, but instead exit through the upper end of the pond. Lower wind speed at water level means lower emission uptakes than with 6 m wind speed which was used for AERMOD and HEGADAS-S model analyses. This also means AERMOD and HEGADAS-S potentially overestimated actual emissions with using 6 m wind speed.

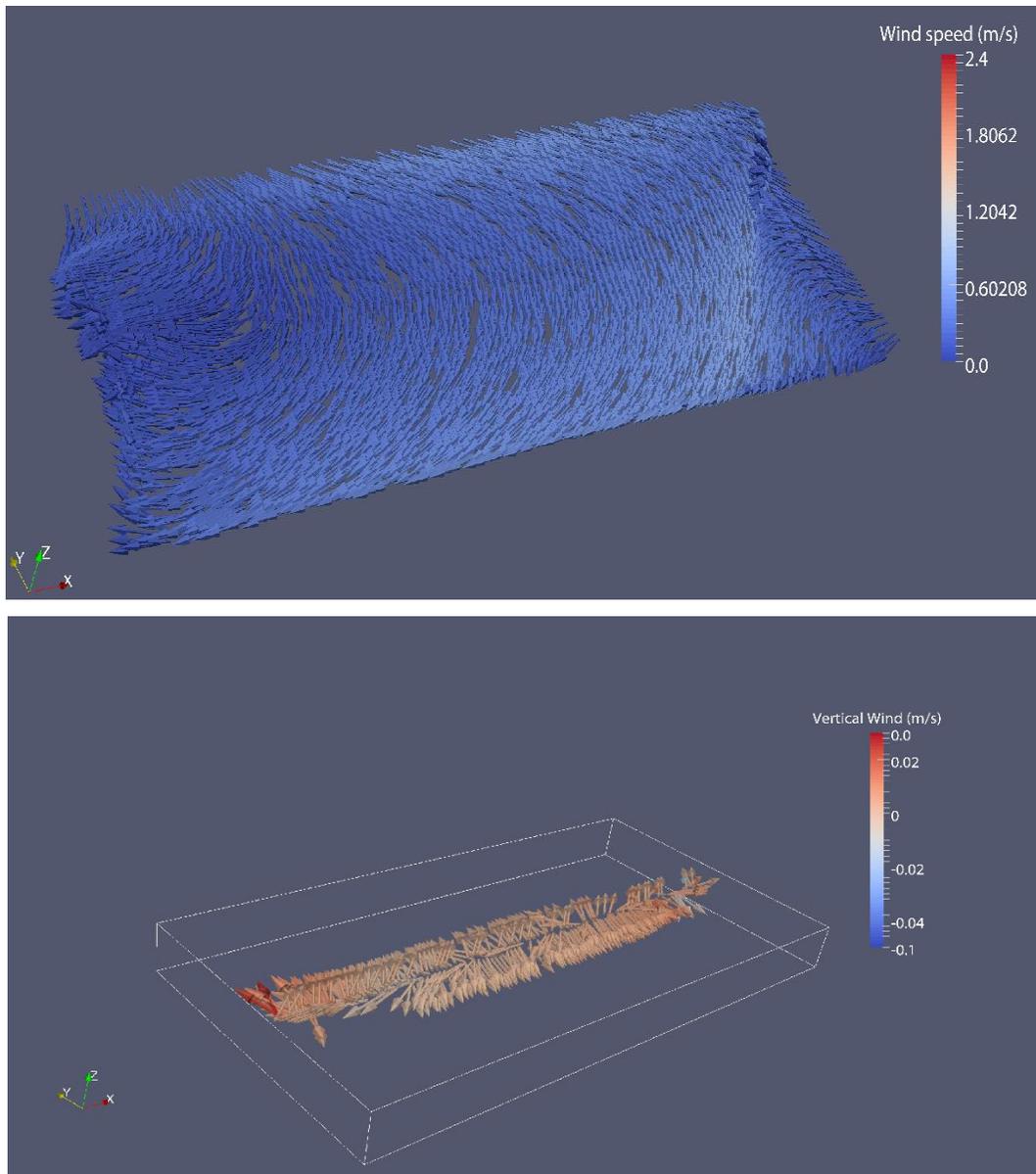


Figure S2. Wind vectors at water level at steady state as simulated by OpenFOAM model (top) and at vertical cross-section along pond's centerline (bottom). The cross-sectional wind vectors are color-coded with magnitude of vertical wind speed component.

Note that due to the high efforts and computational time required to perform fluid dynamic model simulation, we only applied the OpenFOAM analyses for the Case Study. Base on finding with OpenFOAM, we performed full-pond and partial-pond simulation scenarios with HEGADAS-S and examined the results.