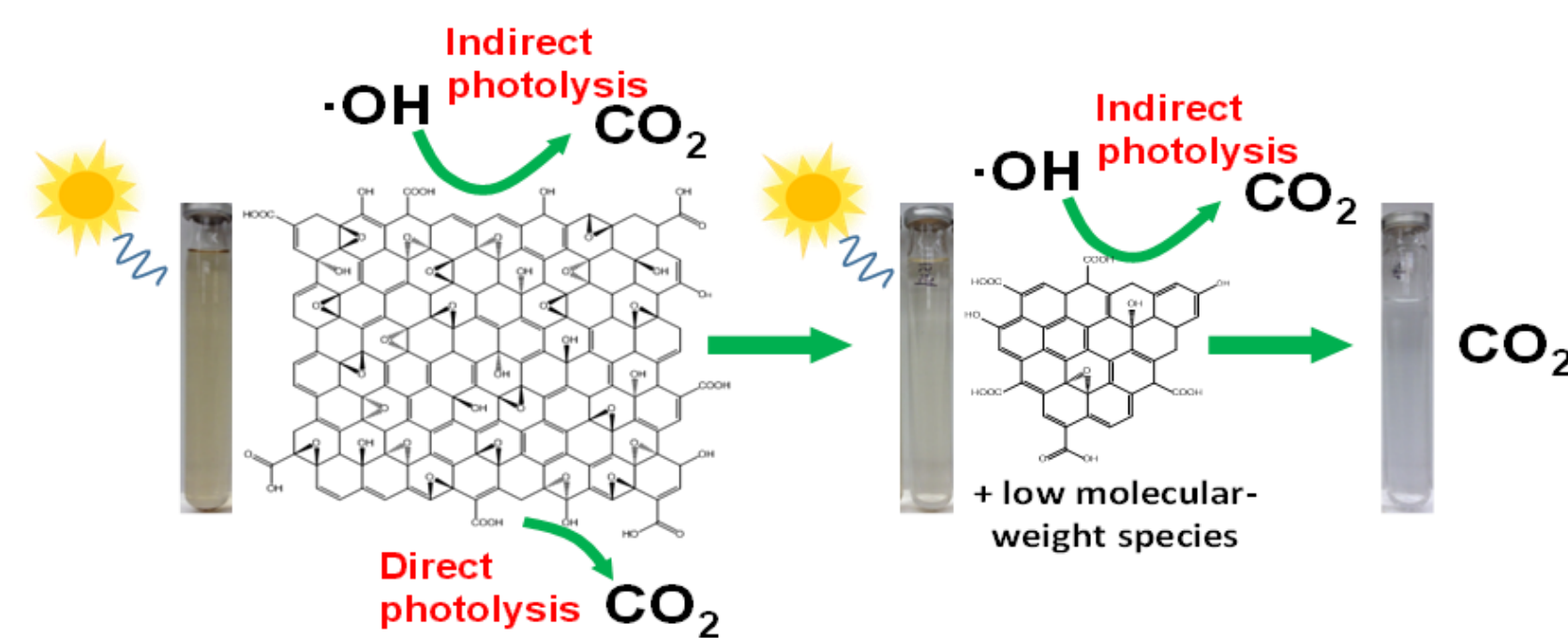


Abstract

The production and potential applications of graphene family nanomaterials may result in unintended releases of these materials into the environment. Like graphene, graphene oxide (GO) exists as 2-dimensional sheets, but GO is much more readily dispersed in water due to the presence of edge carboxyl groups as well as hydroxyl and epoxy groups in the basal plane. After dispersal in a surface water, GO may be transformed under sunlight to yield photoproducts that include oxygenated PAHs. In this work we identify the major PAH photoproducts generated during GO transformation under sunlight using LC/MS-MS. In addition, oxygenated PAH partitioning and speciation in surface waters are estimated, and the Water Quality Analysis Simulation Program (WASP8) is used to simulate potential PAH concentrations in surface waters.

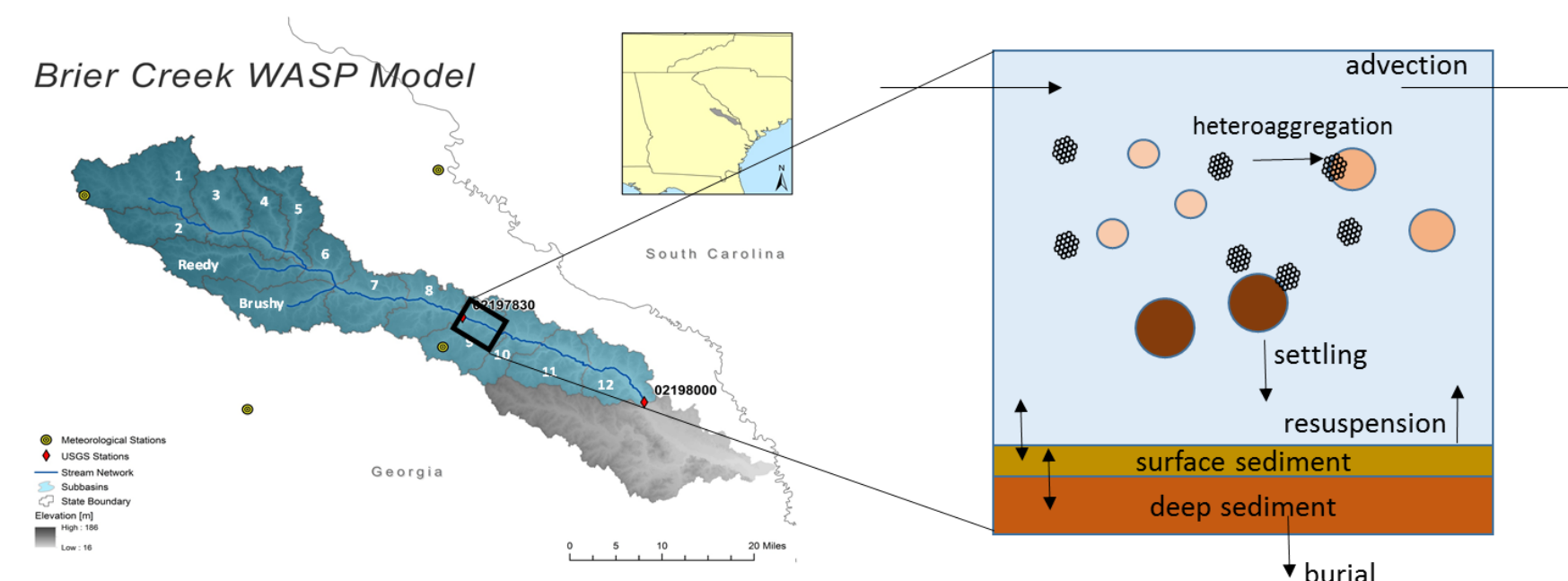
GO Phototransformation



Major GO photoproducts are reduced GO and oxygenated PAHs.

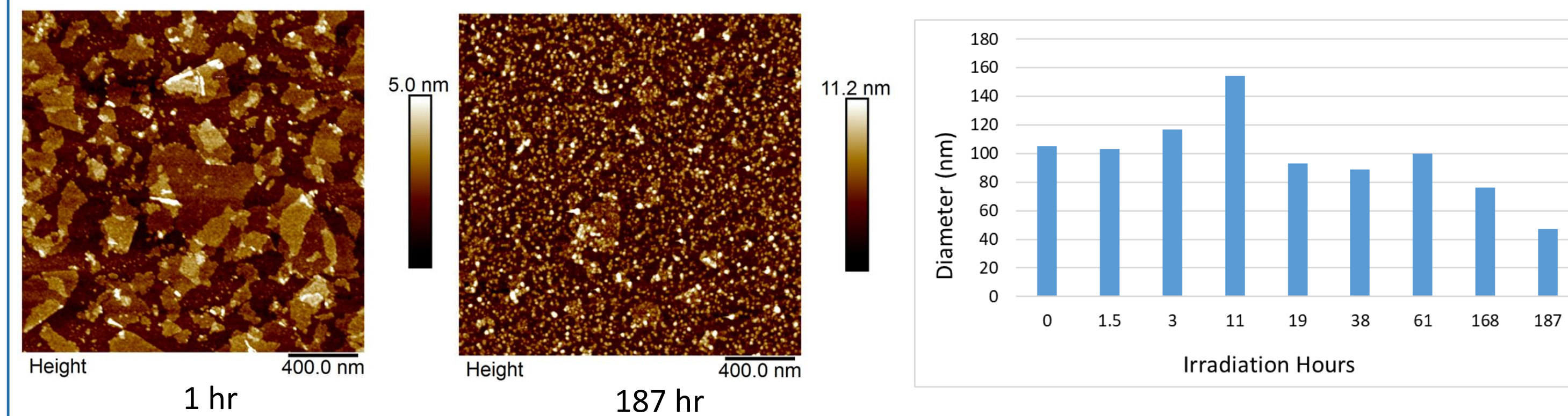
GO Environmental Fate Modeling

WASP8 is a flexible, dynamic, mass-balance framework for developing mechanistic surface water models that simulate the fate of environmental contaminants, including nanomaterials.

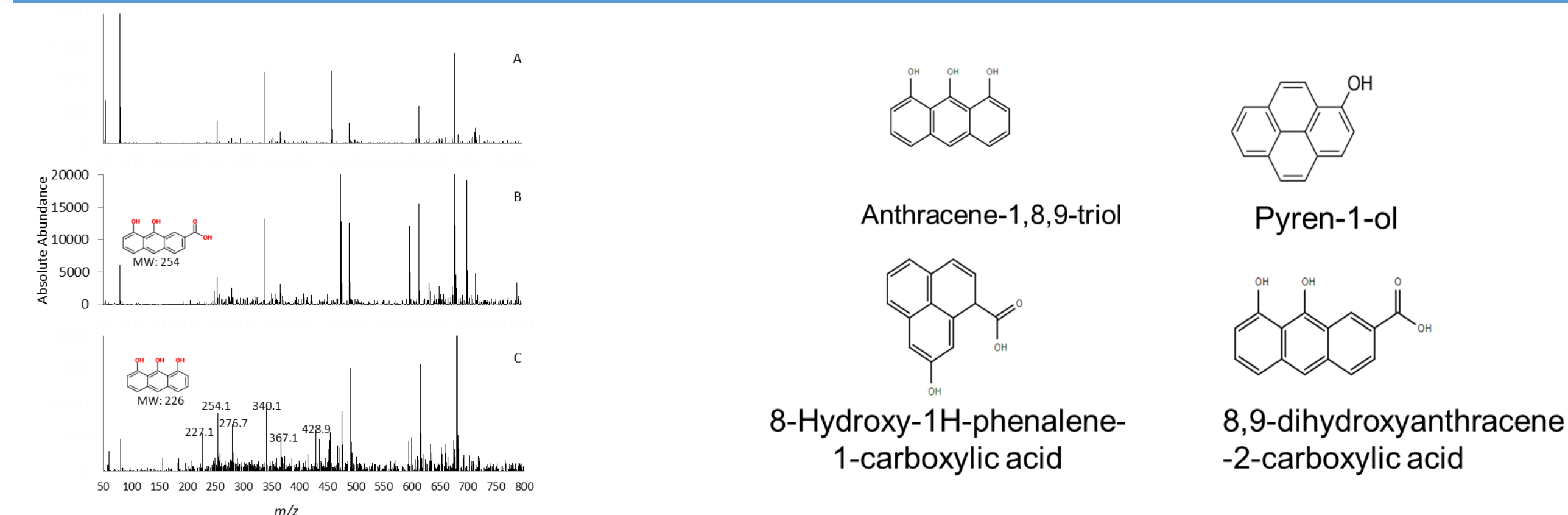


GO Photoproducts

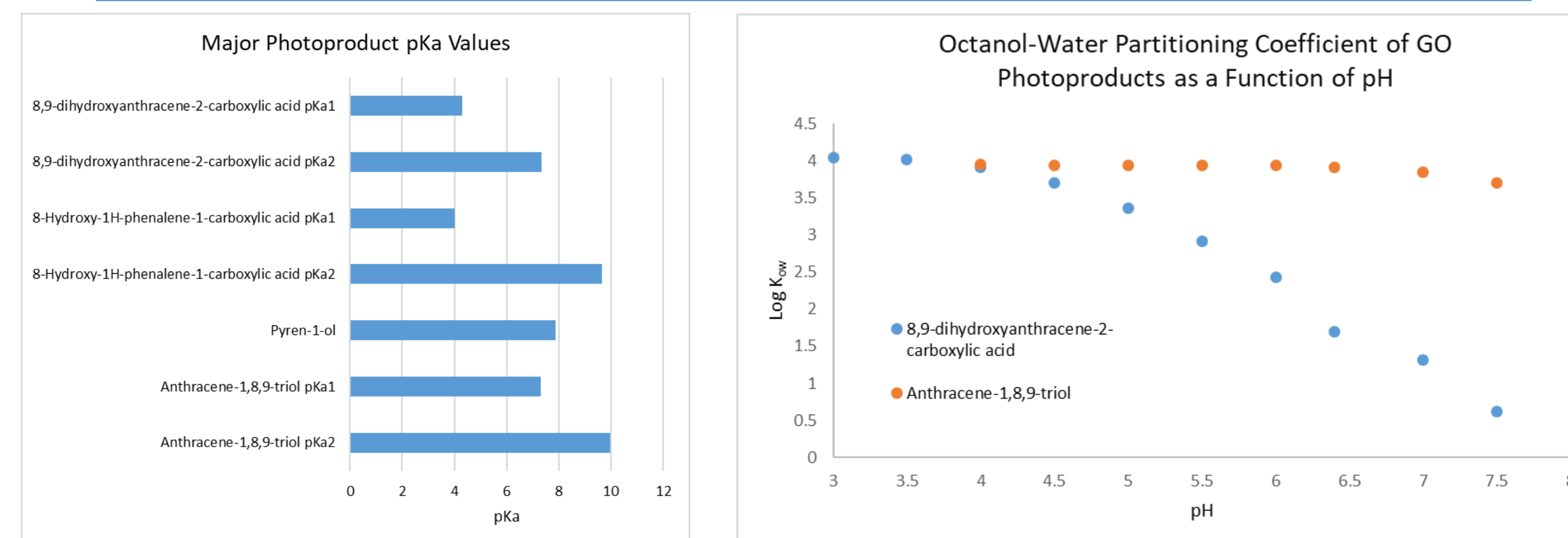
GO AFM Characterization



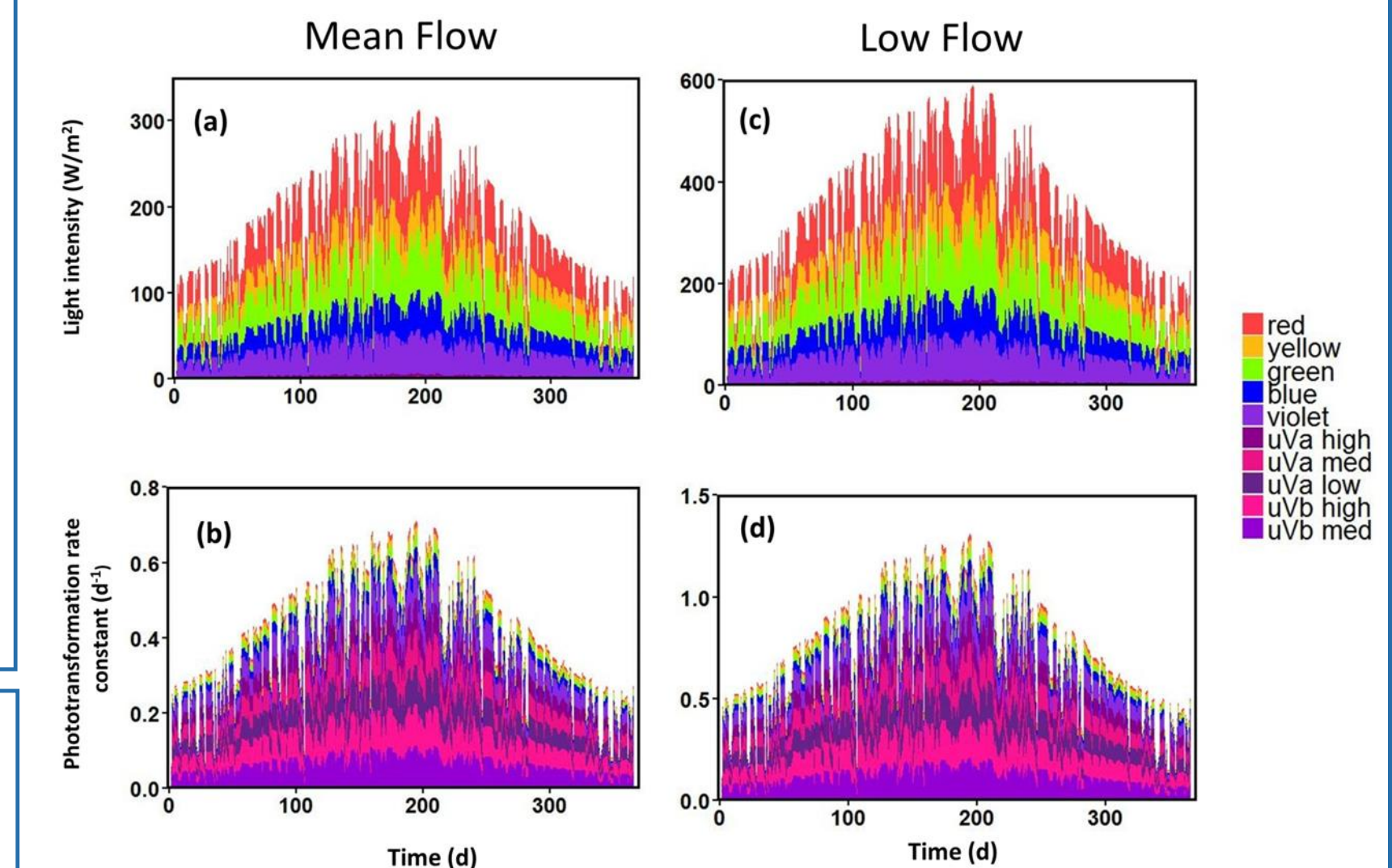
Major PAH Photoproducts



Photoproduct pK_a and K_{ow} Values



Light Attenuation and GO Phototransformation Rates



Daily light intensity and phototransformation rate constants in the first Brier Creek stream segment in 2016

Conclusions

- GO size varied over irradiation time likely reflecting the opposing processes of homoaggregation (size increase) and GO platelet degradation (size decrease).
- pK_{a1} values for the GO photoproducts ranged from 4.02 – 7.88. Log K_{ow} was dependent on pH for PAH's with carboxyl functional groups.
- WASP simulations indicate that PAH photoproduct concentration in the water column was dependent on sunlight intensity: the highest PAH concentrations were observed in the summer months and the lowest concentrations in the winter months.

References

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