

Photo degradation experiment

The experiments were performed in a one-liter quartz round bottom flask (further referred to as "reaction flask") with one liter sample mixed with 0.5 g/L of TiO2 powder (Degussa, P25, Evonik). The chosen catalyst concentration represents a balance under the reasons mentioned below:

1. The conversion rate of the reaction should be sufficient for the appropriate time limits of the experiment (a few hours)

2. The reaction should not proceed so quickly, so that the transformation of the educts (DOM) is complete only in a short period of time, otherwise little to no change of the species in the samples can be quantified nor qualified

3. The catalyst concentration should not exceed a certain threshold to cause such turbidity of the suspension, that would significantly impair the irradiation of the sample. The TiO2 powder was first put to the flasks and the effluent-water was slowly added under stirring (using magnetic stir bar) to avoid agglomeration of the catalyst particles. The irradiating apparatus used was the "UVACUBE 400" from the company "Hönle". The apparatus consisted of a light-insulated cabinet, on top of which sat the lamp, simulating the natural sunlight, separated from the cabinet by a shutter-mechanism. The provided irradiation dose is 28 mW/cm2 at the bottle bottom.



UVACUBE 400 and the emitted spectrum of the irradiating lamp.

For each experiment a total of eight samples at the following timestamps were taken: 0 min, 10 min, 20 min, 30 min, 60 min, 120 min, 180 min and 300 min. The samples were taken directly from the reaction mixture with a syringe, then filtered through polyvinylidene fluoride (PVDF) syringe filters into small 60 mL brown-glass vials. Each filter was conditioned with a few mL of the sample water prior to the filling of the vials. The temperature readings were taken with a clean thermometer submerged directly into the vials. A total volume of the water extracted from the reaction flask was around 480 mL. It is important to note, that the catalyst was extracted from the reaction flask along with the effluent-water, which, given the perfect mixture, should not have increased the catalyst concentration as the reaction progressed.



Examples for reaction time courses

For better understanding of the reactivity classes, examples of RAW versus reaction time plots are provided. In each plot the DI data are provided in addition. The reactivity classes are explained from the LC data (at selected RT).



Examples for reaction time courses, Prod, <Prod, Degr, Degr>



Examples for reaction time courses, IntP, < IntP >, < IntP, IntP >



Examples for reaction time courses, Res, r.n.a.