Modelling of Photoreactors for Water Teatment

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Abstract

Photocatalytic processes are acquiring increasing attention as a mean to exploit solar energy to promote chemical transformations. Numerous applications can be found in the literature on the use of semiconductors for water treatment or to produce renewable fuels. Very challenging applications combine water treatment with the production of fuels. Examples are the photoreduction of CO_2 to liquid chemicals (HCOOH, HCHO and CH_3OH) and gaseous fuels (CH_4 + H_2). In the same frame, the research is focusing on the valorisation of waste or renewably derived organic compounds in water, to be used as sacrificial agents to achieve hydrogen production during water treatment. At last, water treatment from emerging organic pollutants (e.g. drugs and their metabolites, especially nitrogen containing ones), has serious limitations for the removal efficiency in conventional biological treatment plants, offering an additional driver to the development of advanced water treatment processes that include hydrogen production.

These topics are usually addressed from the point of view of material science, in the search of very specific, often naïve, materials for each reaction. On the contrary, process design is very poorly addressed, with few literature outcomes with respect to catalyst development. Therefore, attention is here paid on reactor design and modelling, to set the basis for the possible scale up of the technology.

We have set up and compared three different types of photoreactors for the three mentioned applications (photoreduction of CO_2, H_2 production coupled with water treatment and the removal of nitrogen containing pollutants from water). Two are made of glass with transparent quartz windows (ca. 300 mL internal volume for materials screening): the former is an annular reactor, where the lamp is immersed in the reacting mixture, the latter has an external lamp, irradiating from the top of the reactor (easier for application with solar light). A third reactor is made of stainless steel, with internal lamp, reacting volume ca. 1.3 L and allows to operate up to the pressure of 20 bar, which is an unexplored high value for photocatalytic applications.

For all the applications we have modelled the radiation flow depending on reactor geometry. This allows to include photons in a kinetic model as “quasi-reactants”. This approach would allow to obtain a suitable kinetic model for the scale-up of the reactor. Indeed, by proposing a scaled-up reactor configuration, adding a radiation pattern, the integration of the kinetic model allows the prediction of reactor productivity and its sizing.

Tests have been carried out also on samples of real waste water, monitoring the conversion of COD and N-containing pollutants in a 10 L pilot photoreactor, in collaboration with ISWA (Stuttgart, Germany, which is gratefully acknowledged).

The choice of a proper reactor configuration and the optimisation of the operating conditions, exploring also unconventional ones, such as high temperature and pressure, allowed to obtain conversions and productivities much higher than what reported in the literature (up to 2 orders of magnitude).