Photocatalytic Reaction Engineering for Solar Water Detoxification

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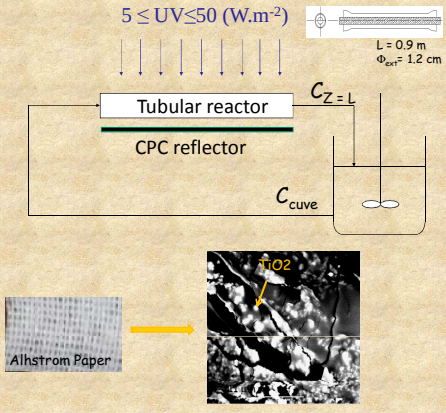
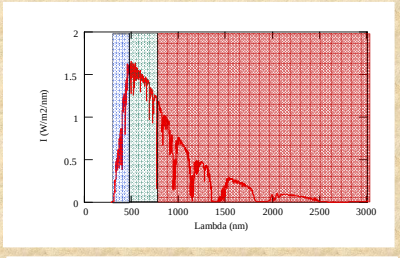
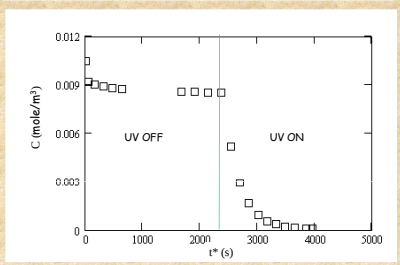
Abstract

Heterogeneous photocatalysis is an alternative method for the removal of organic pollutants in water. The photo excitation of a semi-conductor under ultra violet (UV) irradiation entails the production of hydroxyl radicals, one of the most oxidative chemical species. Combined with solar energy this process of water detoxification is in perfect agreement with the requirement of sustainable processes development. In the open literature, papers have already demonstrated the practical ability of photocatalysis method for the degradation of biorecalcitrant pesticides and more particularly atrazine. With the global objective to design large scale solar water treatment plants, a necessary initial step is the development of a reliable photocatalytic reactor model. Evolution of the concentration of atrazine as a function of the time is measured in a closed fluid loop connecting the tubular reactor and a vessel of atrazine. From these results an original model was developed. It is based on the coupling between: mass transfer from the liquid phase to the surface of the catalyst; adsorption of the pollutant molecules by TiO_2; photocatalytic reaction rate. The validated model is a tool readily usable for reactor design and scale-up.

Experimentation







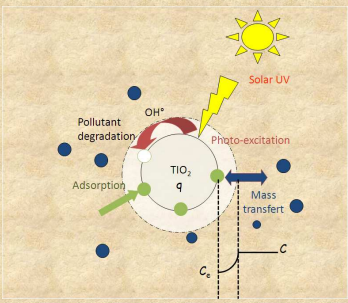
Solar ressource.

Solar spectrum for 1.5 Atmospheric mass (ASTM standard) : 922 W.m^{-2}

- 40 % near IR : 375 W. m^{-2}
- 55 % visible light: 504 W. m^{-2}
- 5 % UV : 43 W. m^{-2}

Atrazine concentration profil in the fluid loop

Modeling at the TiO_2 particules scale



Constitutive equations of the model

$$\frac{\partial C}{\partial t} = -k_f \, S_{cat} \cdot (C - C_e) - u \frac{\partial C}{\partial x}$$

$$\frac{\partial q}{\partial t} = k_f \cdot (C - C_e) - \alpha \cdot I \cdot q$$

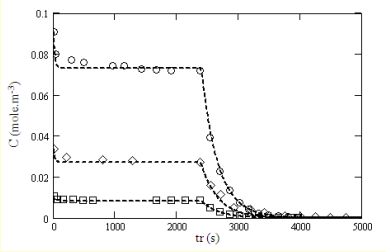
$$\frac{\partial C_{cuve}}{\partial t} = \frac{\dot{m}_v}{V_{cuve}} \cdot (C_{(z=L)} - C_{cuve})$$

$$q = H_{ads} \cdot C_e$$ given by the adsorption isotherm

With:
C atrazine concentration in the bulk phase (mole.m^{-3})
C_e concentration in equilibrium with the adsorbed phase (mole.m^{-3})
C_{cuve} concentration inside the cuve (mole.m^{-3})
q adsorbad quantity of atrazine (mole.m^{-2})
S_{cat} catalyst surface (m^2.m^{-3})
V_{cuve} cuve volume (m^3)
m débit de solution (m^3.s^{-1})
u fluid rate in the reactor (m.s^{-1})

Two parameters :
k_f mass transfer coefficient (m.s^{-1})
α Catlayst efficiency (J.m^{-2})

Atrazine concentration profils with 3 different intial concentrations.



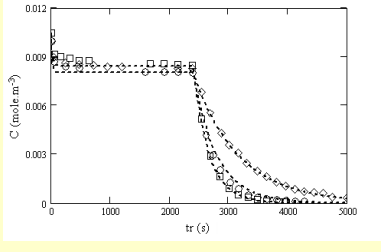
$\dot{m}_v = 0.5\, l.mn^{-1}; UV = 32\, W.m^{-2}$

Results and conclusion

Figures show the comparison between the experimental concentrations and the calculated values (dashed lines) for, respectively different inital concentrations (on the left) and UV irradiations (on the right).
General good agreement whatever are the conditions with :
k_f = 1.65 10^{-5} (m.s^{-1}), α = 1.15 10^{-4} (J.m^{-2})

- Effective coupling phenomena between mass transfert/adsorption/rate of photocatalysis on the adsorbed species.
- First step for a dimensioning tools for solar photocatalysis process.

Atrazine concentration profils with 3 different UV irradiations. (UV = 32, 18, 8 W.m^{-2})



$\dot{m}_v = 0.5\, l.mn^{-1}; C_{init} = 0.01\, mole.m^{-3}$