

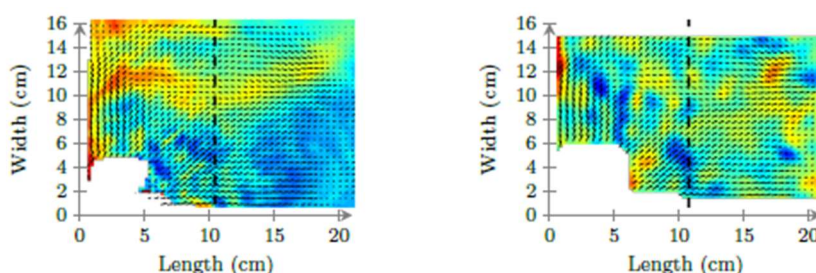
## Characterization of thermally-driven density currents at waterbody / wetland interfaces

### Summary

The occurrence of pharmaceutical compounds in surface waters has been reported worldwide (Al-Odaini et al., 2013; de Jongh et al., 2012; Kolpin et al., 2012; Schwab et al., 2005), with wastewater treatment plants being the main source of these contaminants (Focazio et al., 2008; Nikolaou et al., 2007). These substances arrive at wastewater treatment plants either as parent compounds or as metabolites (Heberer, 2002), via human excretions or deliberate disposal. Despite the chemical and biological processes applied in these facilities, some research works have shown that pharmaceuticals are not often eliminated (Chèvre, 2014; Daughton and Ternes, 1999; Osorio et al., 2012). The fate and transport of pharmaceuticals in the receiving aquatic environment will depend on both biotic and abiotic factors, such as temperature, amount, intensity and wavelength of sunlight, salinity, pH, sediments and flow rate (Fatta-Kassinos et al., 2011). These factors will have influence on transformation processes, like photolysis or biodegradation (Bartels and Von Tümpling, 2007; Winkler et al., 2001), on transport processes between different environmental compartments, like sorption-desorption processes, (da Silva et al., 2011; Kwon and Armbrust, 2008) and on advective and diffusive transport (Bayen et al., 2013). Several investigations showed that the presence of these contaminants affects both aquatic ecosystems and public health (Bruce et al., 2010; Huang et al., 2012). This type of water contamination is expected to increase, since its disposal is directly dependent on the already growing pharmaceutical consumption (Scheurer et al., 2009). Regulatory authorities have now begun to raise concerns about these emergent contaminants, bearing in mind the recent studies showing the ecological and human risks associated to the presence of pharmaceuticals in the environment. In the context of the European Water Framework Directive (EWFD) it is now recognized that pharmaceuticals can represent a relevant issue to achieve the good ecological and chemical status for surface water bodies. For the first time since 2013, on the recent EWFD review, three pharmaceutical compounds have been included on the "watch list" for emerging aquatic pollutants (EU, 2013), namely a general commonly used anti-inflammatory drug (diclofenac), which is suspected of killing fish, and two hormonal ingredients (17 alpha-ethinylestradiol and 17 beta-estradiol) that according to European Commission (EC) can disrupt the endocrine system in humans and harm fish reproduction. Since 2011 the World Health Organization has been annually publishing reports concerning the human health risks of exposure to pharmaceuticals via drinking water. According to this organization, there is a need for the development of cost-effective methods to fulfill the gap of knowledge on the behavior of pharmaceutical compounds in receiving waters, supporting the decision makers on prevention and monitoring programs. Development and application of numerical models in environmental impact assessment has become a common practice, being an important tool for predicting the transport and behavior of pollutants in the aquatic environment (Ji, 2008). These models allow the evaluation of environmental issues through assessment of different scenarios continually described in both space and time, although there are few research works employing numerical methods for forecasting pollution by pharmaceutical compounds. Bearing in mind the need for a model that integrates both fate and transport of pharmaceutical contaminants, this work-program is aimed at assembling and validating a simulation tool for this purpose.

### Keywords

Density currents, hydrodynamics, two-layer mathematical model.



*Density, velocity and vorticity fields of shallow flows.*



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