Proposal for Master thesis work

Modelling of diffusional transport in heterogeneous media

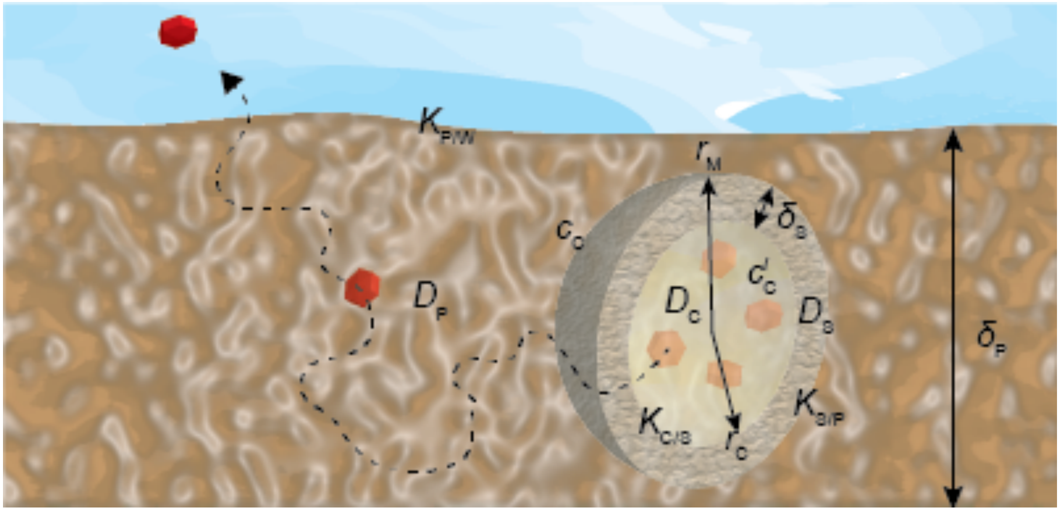

Figure 1 Important parameters for a microencapsulated substance which determine the release rate.

Biocide-containing paint loses the protective ability quite rapidly due to fast biocide leakage. A promising improvement of anti-growth protection can be achieved by the use of encapsulated biocides that slows down the diffusion in the coating. The biocide is placed into microcapsules, from where it is slowly distributed into the surrounding coating matrix.

This project concerns the mechanisms that govern release from microcapsules and the possibility to apply mathematical models that may describe and predict release. The interpretation involves evaluation of the diffusion equation defined to a combined system of various geometries and physicochemical properties. Generated analytical and/or numerical models will be applied on experimental release data.

This thesis work will be performed at the Department of Chemistry and Chemical Engineering (Assoc. Prof. Lars Nordstierna and PhD student Jonatan Bergek) and in close collaboration with Dr. Markus Andersson Trojer at Swerea IVF. The focus will be:

- Theoretical modelling
- Analytical and numerical considerations
- Connection to experimental results

$$\frac{\partial \phi(\boldsymbol{r},t)}{\partial t} = \nabla[D(\phi,\boldsymbol{r})\nabla\phi(\boldsymbol{r},t)]$$

$$\frac{m(t)}{m_{\mathrm{TOT}}} = 1 - 6\frac{6}{\pi^2}\sum_{n=1}^{\infty}\frac{1}{n^2}\exp\left\{-\frac{Dn^2\pi^2 t}{r^2}\right\}$$

Figure 2 The diffusion equation and its solution for release from a monolithic sphere.

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