Numerical software general approach

SURF has a long tradition in developing its own finite element software to simulate electrochemical processes.

In the beginning the models were describing the global current density distributions in electrochemical cells. It is assumed that the bath conductivity is constant and that the polarization can be described by a non-linear function between the current density and the local potential difference between the electrode (V) and the solution (U). Depending on the polarization resistance the so called primary and secondary current density distribution is obtained. This is applied with success in plating processes and cathodic protection (See figure 1).

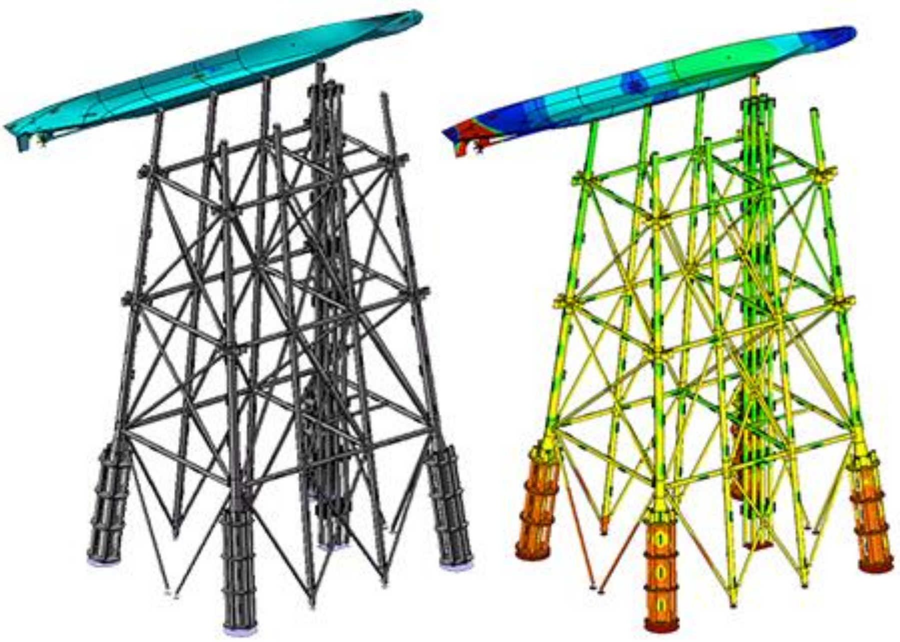
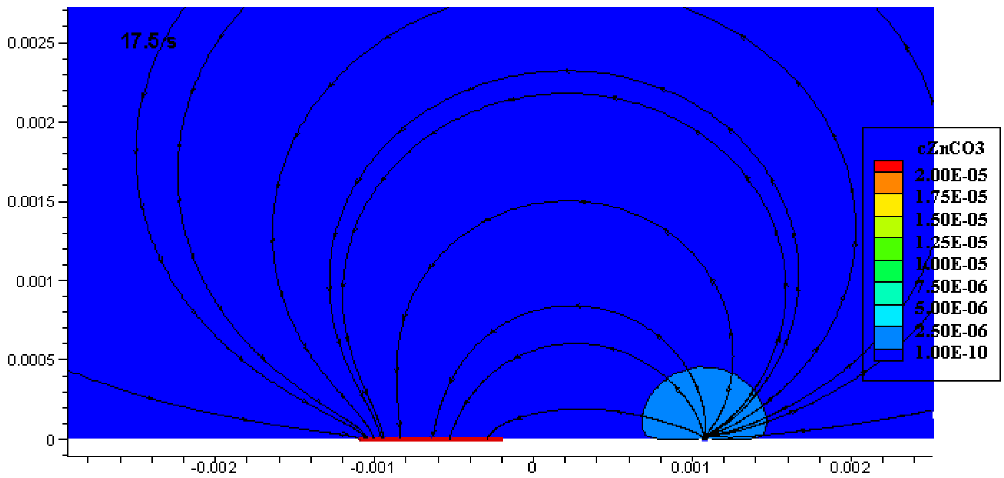


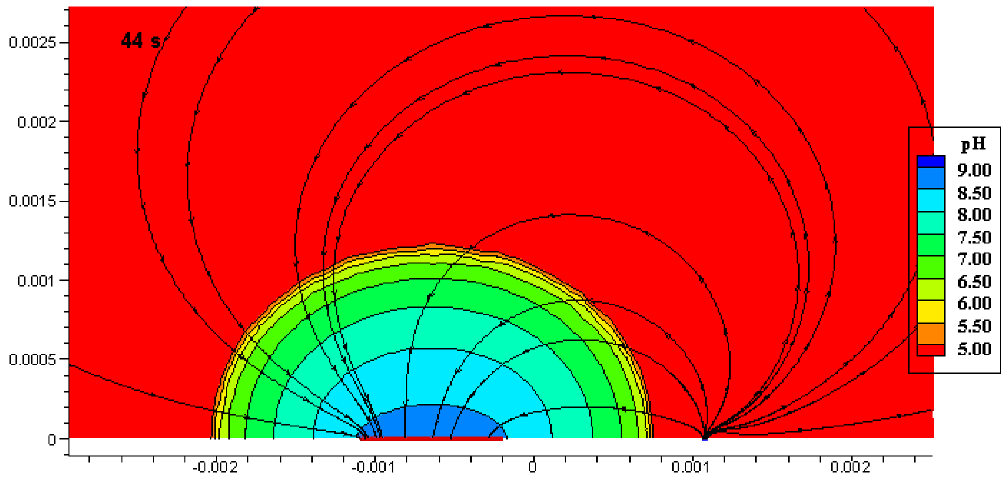
Figure 1: cathodic protection of oil platform and ship hull, each with its own protection system. The oil platform uses sacrificial anodes whereas the ship hull is using mainly impressed current anodes (courtesy Elsyca).

Nowadays the software can handle much more aspects that affect an electrochemical process: fluid flow, mass transfer, heat transfer, adsorption and (electro)chemical kinetics. The program is designed to offer great flexibility towards building models. Today we use these modeling tools in research to obtain quantified understanding of the processes that are occurring. Model reactors (such as the rotating disc cell) are simulated to build and quantify an appropriate electrochemical model. We focus mainly on electrochemical machining and corrosion. Simulations provide in time concentration (Me^{Z+}, Cl^-, etc.), pH, current density and potential distributions. Comparison with measurements provides quantitative data.

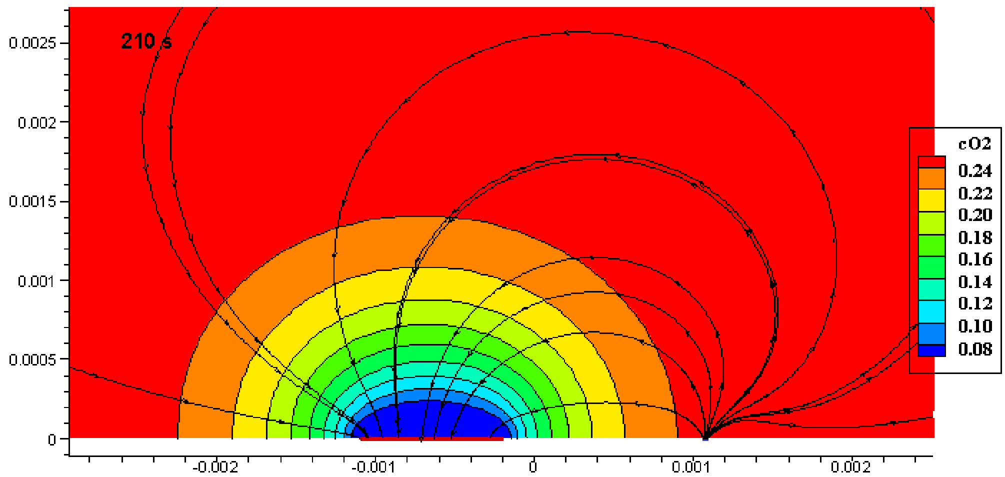
Below one can see some movies on the evolution of the pH, the Zn^{++} and O_2 concentration when a larger iron strip in contact with a small zinc strip. After some time the corrosion rate is reduced due to precipitation of reaction products.



The Zn ions go into the solution whereas the iron is cathodically protected.



The iron is protected by the zinc oxidation. The pH above the iron increases as oxygen is reduced.



The oxygen consumption is resulting in the formation of a boundary layer. Mass transfer of oxygen controls the corrosion rate.