A transport-based one-dimensional mechanistic model of uniform CO2 corrosion of carbon steel

Abstract

Numerous prediction models for CO2 corrosion of carbon steel exist. Most of these are semi-empirical, while some of the more recent models are based on mechanistic descriptions of the processes underlying CO2 corrosion. A thorough review of the field of CO2 corrosion modeling has been published in 1997. The present study describes another attempt at mechanistic modeling in which some of the deficiencies noted in the previously published works are addressed. The significance of the present study is that it mathematically models most of the important processes present in corrosion using fundamental physico-chemical laws. Therefore, even if the model was primarily created to cover the area of uniform CO2 corrosion, it can, with small modifications, be adapted to cover various other types of corrosion, by addition/removal of species and corresponding chemical and electrochemical reactions.

The model covers: electrochemical reactions at the steel surface, diffusion of species between the metal surface and the bulk including diffusion through porous surface films, migration due to establishment of potential gradients and homogenous chemical reactions including precipitation of surface films. The model can predict the corrosion rate, the growth and morphology of a surface film as well as the concentration and flux profiles for all species involved. For n species in the solution, one has n+1 equations, that is: one transport equation for each species and an equation for the potential. Since all the equations are strongly and non-linearly coupled through the chemical reaction and migration terms, they all have to be solved simultaneously, together with the boundary conditions including the nonlinear surface charge balance equation. The differential transport equations were discretized using a finite difference method and a non-uniform grid. All the nonlinear terms: the fluxes, the chemical reaction rate terms and all the terms in the surface charge balance equation are linearized in variable space. This is achieved by using Taylor series expansion around the known solution and by keeping only the constant and the linear term. The model was implemented in Fortran programming language to increase the speed of the lengthy calculations. The user interface was programmed in Microsoft Excel/Visual Basic in order to exploit the user-friendly features of this package including input/output dialogs and plotting capabilities

Comparisons with laboratory experiments have revealed the strengths of the model such as its ability to assist in understanding of the complex processes taking place during corrosion in the presence of surface films.