

MAE 770 Written Preliminary Exam #1

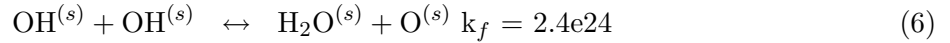
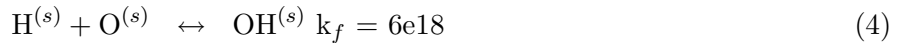
I. Catalytic reaction processes may be modeled by imposing the boundary condition

$$\rho D_k \frac{\partial Y_k^{(g)}}{\partial x_j} \cdot \hat{n}_j = M_k \dot{s}_k \quad (1)$$

in place of the non-catalytic condition

$$\rho D_k \frac{\partial Y_k^{(g)}}{\partial x_j} \cdot \hat{n}_j = 0$$

In this, M_k is the molecular weight and \dot{s} is a source term for surface reactions, which will be a function of concentrations of gas-phase species (g) and surface species (s). The reaction rates for surface reactions are formulated using the law of mass action in the same way as is done for gas-phase reactions, except that concentrations for surface-adsorbed species (s) are expressed as moles/area² as opposed to moles/area³. Concentrations of surface-adsorbed species are also generally expressed as the product of a surface coverage Θ_i and a surface site density Γ (usually a constant). The surface coverage of species i is usually interpreted as the fraction of sites occupied by species i . Now consider the following system of reactions



a.) What are the units of \dot{s}_k and Γ ?

b.) Formulate the source terms \dot{s}_k for k =gas species and k =surface species.

c.) Eq. 1 only holds for gas-phase species participating in surface reactions. In general, what equation holds for surface species participating in surface reactions if the time variation of the surface coverage is held to be zero?

d.) If the forward rate coefficients listed above were determined using a cm, mol, s basis, determine what the forward and backward rate coefficients would be in an SI basis (m, kmol, s).

e.) Explain in detail how one would couple the surface-catalytic equations with a gas-phase CFD code that solves the species conservation equations

$$\frac{\partial \rho Y_k^{(g)}}{\partial t} + \frac{\partial (\rho Y_k^{(g)} u_j - \rho D_k \frac{\partial Y_k^{(g)}}{\partial x_j})}{\partial x_j} = \omega_k$$

, where ω_k is the species production rate for gas-phase reactions, using a finite volume method. Would one expect $\sum_{k=\text{gas species}} \omega_k$ to be zero everywhere in the computational domain?