CHAPTER–VIII

CONCLUSIONS

The solution approach accomplished in this thesis is based on the objective that at the maximum possible level the analytical solutions should be achieved for the model equations, since analytical solutions are the best if available or can be obtained. In the cases where analytical solutions are not achievable or tedious and time consuming, MS Excel iteration technique is desired based upon the model expressions. This approach gives much insight into a system, which is one of the primary objectives of modelling. The use of numerical techniques is preferred only after analytical or semi-analytical approach fails.

- The transient chronoamperometric current for a catalytic reaction mechanism (EC’ reaction) at cylindrical ultra-micro-electrodes using Danckwerts’ expression for small time and small reaction rate was derived and an initial boundary value problem was solved using Danckwerts’ expression.
The analytical solutions for substrate concentration and transient current for both steady and non steady state were obtained using Danckwerts’ relation and variable separable method. A two-point Padé approximation for the non-steady state current for all values of saturation parameter $\alpha$ was also derived.

Approximate analytical solutions of non-linear reaction diffusion equations containing a non linear term related to Michaelis–Menten kinetics of the enzymatic reaction was obtained using variational iteration method.

Numerical solutions for substrate concentration and transient current for non steady state are obtained by finite difference method using MS Excel iteration and a general simple numerical evaluation for current for all values of enzyme saturation parameter were obtained. A moving boundary problem was also solved in MS Excel spread sheet.

A nonlinear ordinary differential equation was solved analytically and the potential time response under Tafel polarization conditions with double layer charging was obtained. The diffusion equations
with linear and non-linear boundaries and with and without double layer effect was solved to obtain the expressions for potential transient using finite difference method in Microsoft excel sheet.

- It was demonstrated that all types of problems can be solved using MS Excel iteration technique.