

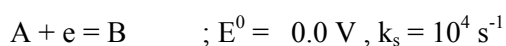
Templates for MECSim input file: Master.inp

Gareth Kennedy, 28/4/2012

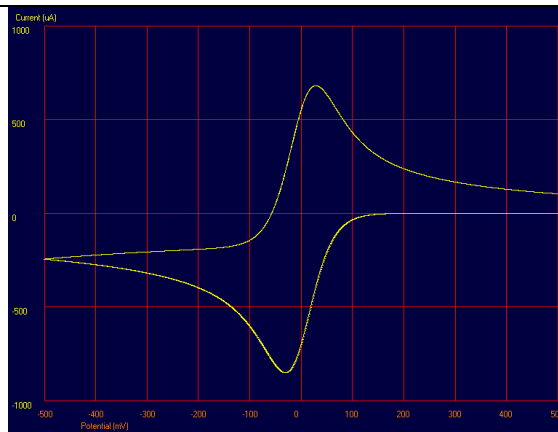
The following examples and associated input file templates will show the user how to set up a range of commonly used mechanisms. This should give the user a good idea of how to edit the Master.inp file to model any desired mechanism. To use one of these templates copy the file (e.g. Master_E.inp) into the same directory as MECSim.exe and rename it Master.inp to run it.

Mechanism 1 (E):

Master_E.inp

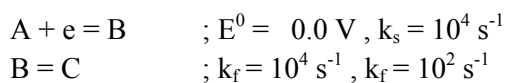


where $[A] = 10^{-6} \text{ mol/cm}^3$.

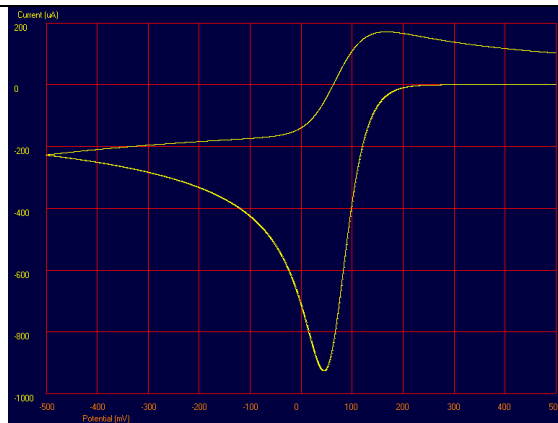


Mechanism 2 (EC):

Master_EC.inp

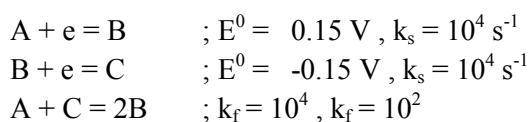


where $[A] = 10^{-6} \text{ mol/cm}^3$.

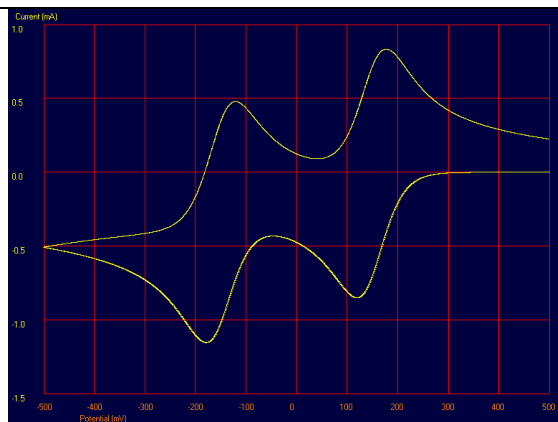


Mechanism 3 (EE):

Master_EE.inp

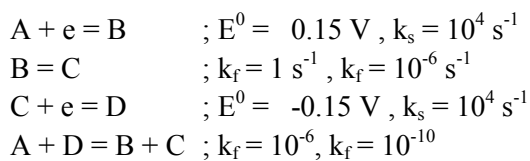


where $[A] = 10^{-6} \text{ mol/cm}^3$ and the rate constants are in units of $\text{cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$.



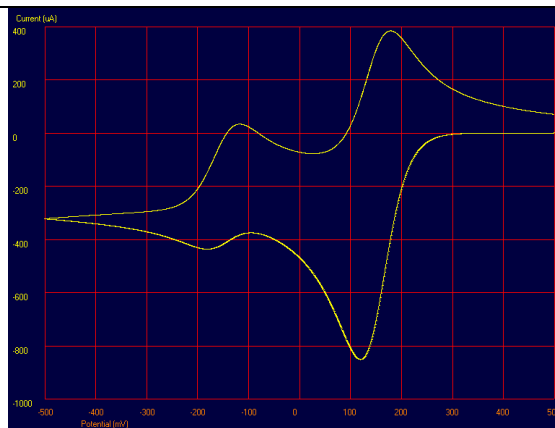
Mechanism 4 (ECE):

Master_ECE.inp

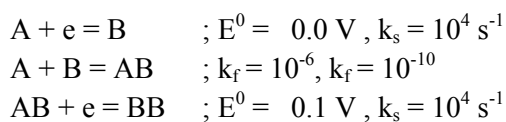


where $[A] = 10^{-6} \text{ mol/cm}^3$ and the second order rate constants are in units of $\text{cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$.

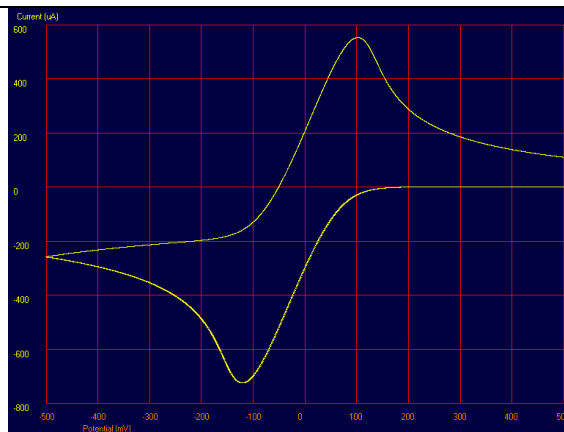
Note that pre-equilibrium is turned off for this mechanism.

**Mechanism 5 (Parent-child):**

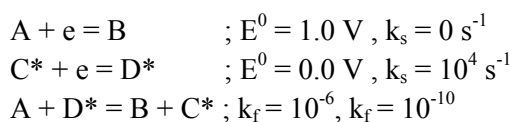
Master_PC.inp



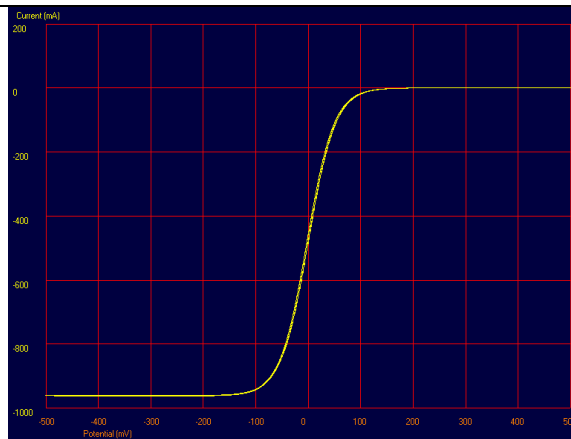
where $[A] = 10^{-6} \text{ mol/cm}^3$ and the rate constants are in units of $\text{cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. In the code AB is the same as C and BB is the same as D. $R_u = 100 \Omega$

**Mechanism 6 (Surface confined catalytic):**

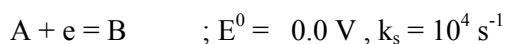
Master_SCCat.inp



where $[A] = 1 \text{ mol/cm}^3$, $[C^*] = 10^{-9} \text{ mol/cm}^3$ and the rate constants are in units of $\text{cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. The first of these electron transfer reactions is used to ensure the correct total current, if not included MECSim will recommend one to use.

**Mechanism 7 (EAC):**

Master_EAC.inp



same as the E mechanism above, but with an additional ac sinusoid with amplitude 50 mV and frequency 180 Hz.

