Templates for MECSim input file: Master.inp

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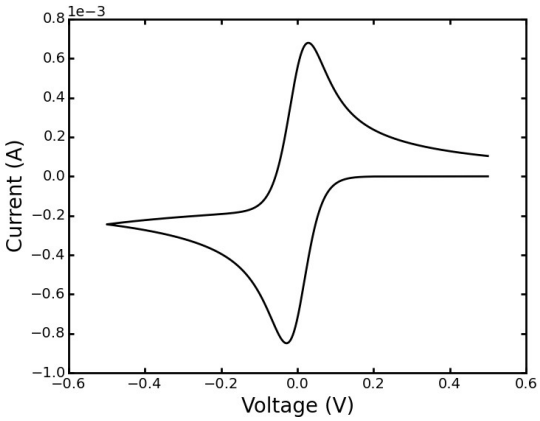
The following examples and associated input file templates will show the user how to set up a range of commonly used mechanisms. This should give the user a good idea of how to edit the Master.inp file to model any desired mechanism. To use one of these templates copy the file (e.g. Master_E.inp) into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

Mechanism 1 (E):
Master_E.inp

A + e = B ; E^0 = 0.0 V , $k_s = 10^4$ s^{-1}

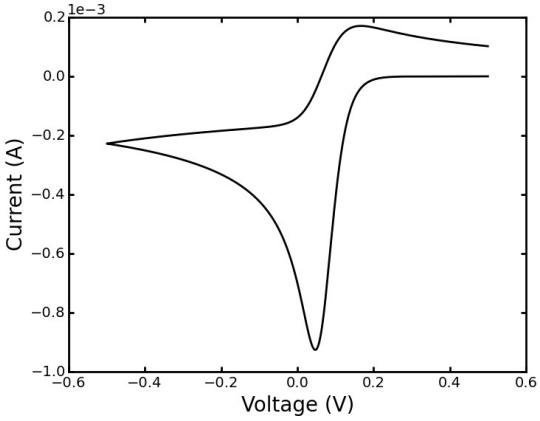
where [A] = 10^{-6} mol/cm^3.



Mechanism 2 (EC):
Master_EC.inp

A + e = B ; E^0 = 0.0 V , $k_s = 10^4$ s^{-1}
B = C ; $k_f = 10^4$ s^{-1} , $k_f = 10^2$ s^{-1}

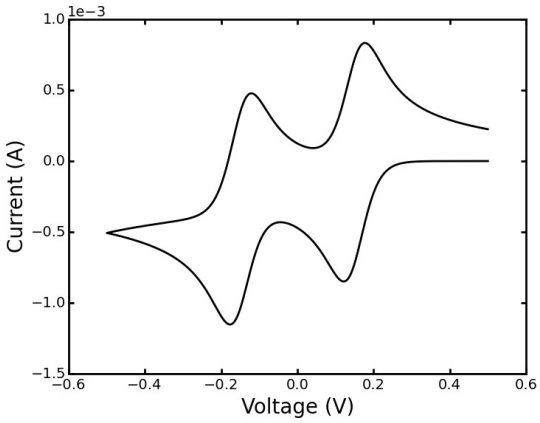
where [A] = 10^{-6} mol/cm^3.



Mechanism 3 (EE):
Master_EE.inp

A + e = B ; E^0 = 0.15 V , $k_s = 10^4$ s^{-1}
B + e = C ; E^0 = -0.15 V , $k_s = 10^4$ s^{-1}
A + C = 2B ; $k_f = 10^4$, $k_f = 10^2$

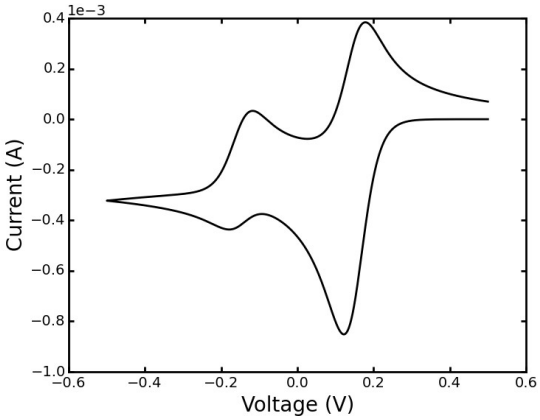
where [A] = 10^{-6} mol/cm^3 and the rate constants are in units of cm^3 mol^{-1} s^{-1}.



Mechanism 4 (ECE):
Master_ECE.inp

A + e = B ; E^0 = 0.15 V , $k_s = 10^4$ s^{-1}
B = C ; $k_f = 1$ s^{-1} , $k_f = 10^{-6}$ s^{-1}
C + e = D ; E^0 = -0.15 V , $k_s = 10^4$ s^{-1}
A + D = B + C ; $k_f = 10^{-6}$, $k_f = 10^{-10}$

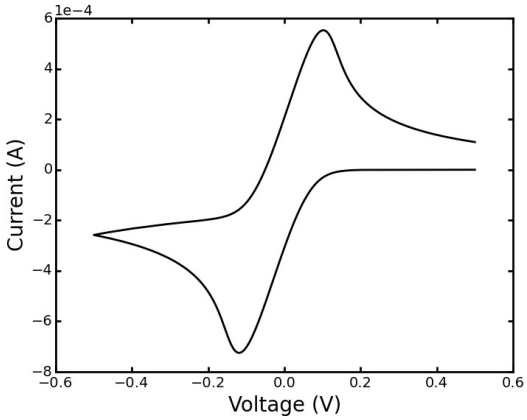
where [A] = 10^{-6} mol/cm^3 and the second order rate constants are in units of cm^3 mol^{-1} s^{-1}.
Note that pre-equilibrium is turned off for this mechanism.



Mechanism 5 (Parent-child):
Master_PC.inp

A + e = B ; E^0 = 0.0 V , $k_s = 10^4$ s^{-1}
A + B = AB ; $k_f = 10^{-6}$, $k_f = 10^{-10}$
AB + e = BB ; E^0 = 0.1 V , $k_s = 10^4$ s^{-1}

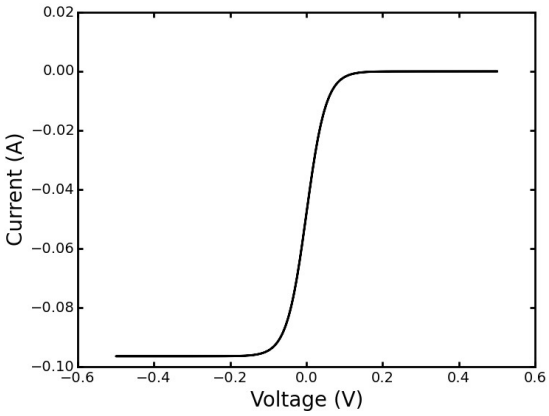
where [A] = 10^{-6} mol/cm^3 and the rate constants are in units of cm^3 mol^{-1} s^{-1}. In the code AB is the same as C and BB is the same as D. **R_u = 100 Ω**



Mechanism 6 (Surface confined catalytic):
Master_SCCat.inp

A + e = B ; E^0 = 1.0 V , k_s = 0 s^{-1}
C* + e = D* ; E^0 = 0.0 V , k_s = 10^4 s^{-1}
A + D* = B + C* ; k_f = 10^{-6}, k_f = 10^{-10}

where [A] = 1 mol/cm^3 ,[C*] = 10^{-9} mol/cm^3 and the rate constants are in units of cm^3 mol^{-1} 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

A + e = B ; E^0 = 0.0 V , k_s = 10^4 s^{-1}

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