

```
###*****###
```

```
# Continuity Equation Procedure #
```

```
#Solutions Used
```

```
#DevPsi - the device potential and is the controlling variable for this pde
```

```
#Elec - the electron concentration
```

```
#Hole - the hole concentration
```

```
#Donor - the ionized donors - can be complicated with partial ionization
```

```
#Acceptor - the ionized acceptors - can be complicated with partial ionization
```

```
#Solutions Created
```

```
#Econd - the conduction band edge
```

```
#Eval - the valence band edge
```

```
#Parameters Set
```

```
#DampValue is set to a thermal voltage at toom temperature
```

```
#AbsError is set to 1mV
```

```
#RelError is set to 0.01
```

```
#Parameters Used
```

```
#RelEps is the relative permittivity, and should be in the PDB as a double "$Mat DevPsi RelEps"
```

```
#Affinity is the electron affinity, and should be in the PDB as a double "$Mat Affinity"
```

```
#Eg is the band gap, and should be in the PDB as a double "$Mat Eg"
```

```
#the electronic charge and permittivity of free space
```

```
set q 1.60218e-19
```

```
set eps0 8.854e-14
```

```
# Call this procedure for electron continuity in a material {Mat}
```

```
proc ElecContinuity {Mat} {
```

```
  global Vt
```

```
  pdbSetDouble $Mat Qfn Rel.Error 1.0e-2
```

```
  pdbSetDouble $Mat Qfn Abs.Error 1.0e-2
```

```
  pdbSetDouble $Mat Qfn DampValue 0.025
```

```
  set eqn "ddt(Elec) - ([pdbDelayDouble $Mat Elec mob]) * (Elec+1.0) * grad(Qfn)"
```

```
  pdbSetString $Mat Qfn Equation $eqn
```

```
  set e "([pdbDelayDouble $Mat Elec Ec])"
```

```
  solution add name=Econd solve $Mat const val = ($e)
```

```
  set e "([pdbDelayDouble $Mat Elec Nc]) * exp( -(Econd-Qfn) / ($Vt) )"
```

```
  solution add name=Elec solve $Mat const val = "($e)"
```

```
}
```

```
# Call this procedure for hole continuity in a material {Mat}
```

```
proc HoleContinuity {Mat} {
```

```
  global Vt
```

```

pdbSetDouble $Mat Qfp Rel.Error 1.0e-2
pdbSetDouble $Mat Qfp Abs.Error 1.0e-2
pdbSetDouble $Mat Qfp DampValue 0.025

set eqn "ddt(Hole) - ([pdbDelayDouble $Mat Hole mob]) * (Hole+1.0) * grad(Qfp)"
pdbSetString $Mat Qfp Equation $eqn

set e "([pdbDelayDouble $Mat Hole Ev])"
solution add name=Eval solve $Mat const val = ($e)

set e "([pdbDelayDouble $Mat Hole Nv]) * exp( -(Qfp - Eval) / ($Vt) )"
solution name=Hole solve $Mat const val = "($e)"
}

# Call this procedure when solving a transient simulation with donor traps with energy {Etrap} and
lifetime {tau} and concentration {Ntrap}
proc ElecContinuity_trans {Mat Ntrap Etrap tau} {
  global Vt

  pdbSetDouble $Mat Qfn Rel.Error 1.0e-2
  pdbSetDouble $Mat Qfn Abs.Error 1.0e-2
  pdbSetDouble $Mat Qfn DampValue 0.025

  set kr "(1/$tau)"

  set kf "($kr * 2 / [pdbDelayDouble $Mat Elec Nc] * exp( $Etrap / ($Vt)))"
  #set kr "($kf * [pdbDelayDouble $Mat Elec Nc] / 2 * exp(- $Etrap / ($Vt)))"

  set eqn "ddt(Elec) - ([pdbDelayDouble $Mat Elec mob]) * (Elec+1.0) * grad(Qfn) + ($kf * (Donor * Elec))
- ($kr * ($Ntrap - Donor))"
  pdbSetString $Mat Qfn Equation $eqn

  set e "([pdbDelayDouble $Mat Elec Ec])"
  solution add name=Econd solve $Mat const val = ($e)

  set e "([pdbDelayDouble $Mat Elec Nc]) * exp( -(Econd-Qfn) / ($Vt) )"
  solution add name=Elec solve $Mat const val = "($e)"
}

```

```

# Call this procedure when solving a transient simulation with donor traps with energy {Etrap} and
lifetime {tau} and concentration {Ntrap}
proc DonorContinuity_trans {Mat Ntrap Etrap tau} {
  global Vt

  pdbSetDouble $Mat Donor Rel.Error 1.0e-2
  pdbSetDouble $Mat Donor Abs.Error 1.0e-2
  pdbSetDouble $Mat Donor DampValue 0.025

```

```
set kr "(1/$tau)"
```

```
set kf "($kr * 2 / [pdbDelayDouble $Mat Elec Nc] * exp( $Etrap / $Vt))"
```

```
#set kr "($kf * [pdbDelayDouble $Mat Elec Nc] / 2 * exp(- $Etrap / ($Vt)))"
```

```
set eqn "ddt(Donor) + ( $kf * (Donor * Elec)) - ($kr * ($Ntrap - Donor))"
```

```
pdbSetString $Mat Donor Equation $eqn
```

```
}
```

```
solution name=Hole Gas const val=0.0
```

```
solution name=Eval Gas const val=0.0
```