! Hydrogen desorption

program Hdesorption

implicit none

interface

subroutine FDM(Hl,Hs,D,dz,dt,grid)

integer :: i, grid

real(8), allocatable, dimension(:) :: Hl,Hl\_update

real(8) :: Hs,D,dz,dt

end subroutine FDM

subroutine FDM\_s(Hl,Hs,D,dz,dt,z,grid)

integer :: i, grid

real(8), allocatable, dimension(:) :: Hl, z, Hl\_update

real(8) :: Hs,D,dz,dt

end subroutine FDM\_s

subroutine local\_eq(Hl,Ht,Nl,Nt,k,T)

real(8) :: Hl,Ht,Nl,Nt,Eb,k,T

real(8) :: y1,y2,y3,gl,gt,total

end subroutine local\_eq

subroutine kinetic(Hl,Ht,Nl,Nt,Q,Eb,dt,T)

real(8) :: Hl,Nl,Ht,Nt,Q,Eb,dt,T

real(8) :: Ht\_up,Hl\_up, Ptl, Plt

real(8) :: prob

end subroutine kinetic

end interface

integer :: i,icharge,iage,ishape,mode,iter,grid

real(8), allocatable, dimension(:) :: Hl, z, Ht1, Ht2, Ht3, area\_f

real(8) :: Hs,dz,dt,D0,Q,l,D,Nl

real(8) :: avel,ave1,ave2,ave3

real(8) :: Eb1,Eb2,Eb3,Nt1,Nt2,Nt3

real(8) :: k1,k2,k3

real(8) :: ch\_time,ag\_time,des\_time,T,Tend,dTdt,time,time1

real(8), parameter :: R=8.3144621d0 !Gas constant J/mol

real(8), parameter :: Mu=1d13 !Prefactor

real(8), parameter :: Na=6.02214129d23 !Avogadro mol^-1

real(8), parameter :: mass=55.845 !Fe atomic weight

real(8), parameter :: Vm=7.09e-6

!

namelist /specimen/ D0,Q,l,Hs,Eb1,Eb2,Eb3,Nl,Nt1,Nt2,Nt3

namelist /analysis/ mode,ch\_time,ag\_time,des\_time,dt,T,Tend,dTdt

namelist /option/ icharge, iage, ishape,grid

! Read input file "in.txt"

open(unit=1,file='in.txt',status='old')

read(1,specimen)

read(1,analysis)

read(1,option)

close(1)

! Allocation of Hl, z, Ht1, Ht2, Ht3, area\_f

allocate(Hl(grid))

allocate(z(grid))

allocate(Ht1(grid))

allocate(Ht2(grid))

allocate(Ht3(grid))

allocate(area\_f(grid))

! Initialization of all arrays

Hl=0d0

z=0d0

Ht1=0d0

Ht2=0d0

Ht3=0d0

area\_f=0d0

time=0d0

time1=0d0

!

dz=l/grid

z(1)=dz/2

do i=2,grid

z(i)=z(i-1)+dz

enddo

d=d0\*exp(-Q/R/T)

do while (dt>=(dz\*dz/3/d)) !.ge.

dt=dt/2

print \*, 'Too large dt\_FDM 1'

enddo

if (ishape==1) then

area\_f(1)=dz\*dz/l/l

do i=2,grid

area\_f(i)=dz\*dz\*(i\*i-(i-1)\*(i-1))/l/l

enddo

endif

open(unit=10,file='lattice.txt',status='unknown')

Nl=Nl\*Vm/mass/Na\*1e6

if (Nt1.gt.0) then

k1=exp(Eb1/R/T)

Nt1=Nt1\*Vm/mass/Na\*1e6

open(unit=11,file='trap1.txt',status='unknown')

endif

if (Nt2.gt.0) then

k2=exp(Eb2/R/T)

Nt2=Nt2\*Vm/mass/Na\*1e6

open(unit=12,file='trap2.txt',status='unknown')

endif

if (Nt3.gt.0) then

k3=exp(Eb3/R/T)

Nt3=Nt3\*Vm/mass/Na\*1e6

open(unit=13,file='trap3.txt',status='unknown')

endif

do while (time<ch\_time) !.lt.

if (icharge==0) then

open(unit=2,file='charging.txt',status='old')

read(2,\*) z

read(2,\*) Hl

read(2,\*) Ht1

read(2,\*) Ht2

read(2,\*) Ht3

close(2)

goto 10

endif

if (ishape==0) then

call FDM(Hl,Hs,D,dz,dt,grid)

else

call FDM\_s(Hl,Hs,D,dz,dt,z,grid)

endif

if (time1>=des\_time) then !.ge.

write(10,'(F9.0,F7.2, 5000E11.4)') time,T-273,Hl

write(11,'(F9.0,F7.2, 5000E11.4)') time,T-273,Ht1

write(12,'(F9.0,F7.2, 5000E11.4)') time,T-273,Ht2

write(13,'(F9.0,F7.2, 5000E11.4)') time,T-273,Ht3

time1=0d0

endif

do i=1,grid

if (Nt1.gt.0) call local\_eq(Hl(i),Ht1(i),Nl,Nt1,k1,T)

if (Nt2.gt.0) call local\_eq(Hl(i),Ht2(i),Nl,Nt2,k2,T)

if (Nt3.gt.0) call local\_eq(Hl(i),Ht3(i),Nl,Nt3,k3,T)

enddo

time=time+dt

time1=time1+dt

enddo

if (ishape==0) then

avel=sum(Hl)/grid

ave1=sum(Ht1)/grid

ave2=sum(Ht2)/grid

ave3=sum(Ht3)/grid

else

avel=sum(Hl\*area\_f)

ave1=sum(Ht1\*area\_f)

ave2=sum(Ht2\*area\_f)

ave3=sum(Ht3\*area\_f)

endif

write(10,'(F9.0,F7.2, 5000E11.4)') time,T-273,Hl

write(10,\*) '------------------------------------'

write(11,'(F9.0,F7.2, 5000E11.4)') time,T-273,Ht1

write(11,\*) '------------------------------------'

write(12,'(F9.0,F7.2, 5000E11.4)') time,T-273,Ht2

write(12,\*) '------------------------------------'

write(13,'(F9.0,F7.2, 5000E11.4)') time,T-273,Ht3

write(13,\*) '------------------------------------'

!

open(unit=2,file='charging.txt',status='unknown')

write(2,'(500E11.4)') z

write(2,'(500E11.4)') Hl

write(2,'(500E11.4)') Ht1

write(2,'(500E11.4)') Ht2

write(2,'(500E11.4)') Ht3

write(2,'(F9.0,4E11.4)') time,avel,ave1,ave2,ave3

close(2)

!

10 time=0d0

time1=0d0

Hs=0d0

do while (time.lt.ag\_time)

if (iage==0) then

open(unit=3,file='aging.txt',status='old')

read(3,\*) z

read(3,\*) Hl

read(3,\*) Ht1

read(3,\*) Ht2

read(3,\*) Ht3

close(3)

goto 11

endif

if (ishape==0) then

call FDM(Hl,Hs,D,dz,dt,grid)

else

call FDM\_s(Hl,Hs,D,dz,dt,z,grid)

endif

if (time1>=des\_time) then !.ge.

write(10,'(F9.0,F7.2, 5000E11.4)') time,T-273,Hl

write(11,'(F9.0,F7.2, 5000E11.4)') time,T-273,Ht1

write(12,'(F9.0,F7.2, 5000E11.4)') time,T-273,Ht2

write(13,'(F9.0,F7.2, 5000E11.4)') time,T-273,Ht3

time1=0d0

endif

do i=1,grid

if (Nt3.gt.0) call local\_eq(Hl(i),Ht3(i),Nl,Nt3,k3,T)

if (Nt2.gt.0) call local\_eq(Hl(i),Ht2(i),Nl,Nt2,k2,T)

if (Nt1.gt.0) call local\_eq(Hl(i),Ht1(i),Nl,Nt1,k1,T)

enddo

time=time+dt

time1=time1+dt

enddo

if (ishape==0) then

avel=sum(Hl)/grid

ave1=sum(Ht1)/grid

ave2=sum(Ht2)/grid

ave3=sum(Ht3)/grid

else

avel=sum(Hl\*area\_f)

ave1=sum(Ht1\*area\_f)

ave2=sum(Ht2\*area\_f)

ave3=sum(Ht3\*area\_f)

endif

write(10,'(F9.0,F7.2, 5000E11.4)') time,T-273,Hl

write(10,\*) '------------------------------------'

write(11,'(F9.0,F7.2, 5000E11.4)') time,T-273,Ht1

write(11,\*) '------------------------------------'

write(12,'(F9.0,F7.2, 5000E11.4)') time,T-273,Ht2

write(12,\*) '------------------------------------'

write(13,'(F9.0,F7.2, 5000E11.4)') time,T-273,Ht3

write(13,\*) '------------------------------------'

open(unit=3,file='aging.txt',status='unknown')

write(3,'(500E11.4)') z

write(3,'(500E11.4)') Hl

write(3,'(500E11.4)') Ht1

write(3,'(500E11.4)') Ht2

write(3,'(500E11.4)') Ht3

write(3,'(F9.0,4E11.4)') time,avel,ave1,ave2,ave3

close(3)

11 time=0d0

time1=0d0

print \*, '\*\*\*\*\* Start desorption \*\*\*\*\*'

iter=0

open(unit=20,file='results.txt',status='unknown')

write(20,'(F9.2,E11.4)') (T-273), (avel+ave1+ave2+ave3)

do while (T.le.Tend)

if (ishape==0) then

call FDM(Hl,Hs,D,dz,dt,grid)

else

call FDM\_s(Hl,Hs,D,dz,dt,z,grid)

endif

if (time1>=des\_time) then !.ge.

write(10,'(F9.0,F7.2, 5000E11.4)') time,T-273,Hl

write(11,'(F9.0,F7.2, 5000E11.4)') time,T-273,Ht1

write(12,'(F9.0,F7.2, 5000E11.4)') time,T-273,Ht2

write(13,'(F9.0,F7.2, 5000E11.4)') time,T-273,Ht3

if (ishape==0) then

avel=sum(Hl)/GRID

ave1=sum(Ht1)/GRID

ave2=sum(Ht2)/GRID

ave3=sum(Ht3)/GRID

else

avel=sum(Hl\*area\_f)

ave1=sum(Ht1\*area\_f)

ave2=sum(Ht2\*area\_f)

ave3=sum(Ht3\*area\_f)

endif

!write(20,\*) (T-273), avel,ave1,ave2,ave3

write(20,'(F9.2,E11.4)') T-273,avel+ave1+ave2+ave3

time1=0d0

endif

do i=1,grid

if (mode.eq.0) then

if (Nt3.gt.0) call kinetic(Hl(i),Ht1(i),Nl,Nt3,Q,Eb3,dt,T)

if (Nt2.gt.0) call kinetic(Hl(i),Ht2(i),Nl,Nt2,Q,Eb2,dt,T)

if (Nt1.gt.0) call kinetic(Hl(i),Ht1(i),Nl,Nt1,Q,Eb1,dt,T)

else

if (Nt3.gt.0) call local\_eq(Hl(i),Ht3(i),Nl,Nt3,k3,T)

if (Nt2.gt.0) call local\_eq(Hl(i),Ht2(i),Nl,Nt2,k2,T)

if (Nt1.gt.0) call local\_eq(Hl(i),Ht1(i),Nl,Nt1,k1,T)

endif

enddo

do while (dt>=(dz\*dz/3/D)) !.ge.

dt = dt\*0.5

print \*, 'Too large dt\_FDM 2'

enddo

T=T+dTdt\*dt

time=time+dt

time1=time1+dt

iter=iter+1

if (mod(iter,400000).eq.0) write(\*,'(F11.2)') T-273

d=d0\*exp(-Q/R/T)

if (Nt1.gt.0) k1=exp(Eb1/R/T)

if (Nt2.gt.0) k2=exp(Eb2/R/T)

if (Nt3.gt.0) k3=exp(Eb3/R/T)

enddo

if (ishape==0) then

avel=sum(Hl)/GRID

ave1=sum(Ht1)/GRID

ave2=sum(Ht2)/GRID

ave3=sum(Ht3)/GRID

else

avel=sum(Hl\*area\_f)

ave1=sum(Ht1\*area\_f)

ave2=sum(Ht2\*area\_f)

ave3=sum(Ht3\*area\_f)

endif

write(10,'(F9.0,F7.2, 5000E11.4)') time,T-273,Hl

write(10,\*) '------------------------------------'

write(11,'(F9.0,F7.2, 5000E11.4)') time,T-273,Ht1

write(11,\*) '------------------------------------'

write(12,'(F9.0,F7.2, 5000E11.4)') time,T-273,Ht2

write(12,\*) '------------------------------------'

write(13,'(F9.0,F7.2, 5000E11.4)') time,T-273,Ht3

write(13,\*) '------------------------------------'

open(unit=4,file='desorption.txt',status='unknown')

write(4,'(500E11.4)') z

write(4,'(500E11.4)') Hl

write(4,'(500E11.4)') Ht1

write(4,'(500E11.4)') Ht2

write(4,'(500E11.4)') Ht3

write(4,'(F9.0,4E11.4)') time,avel,ave1,ave2,ave3

close(4)

end program Hdesorption

!-------------------------------------------------------------------------------------

subroutine FDM(Hl,Hs,D,dz,dt,grid)

implicit none

integer :: i, grid

real(8), allocatable, dimension(:) :: Hl,Hl\_update

real(8) :: Hs,D,dz,dt

! Allocate temp array

allocate(Hl\_update(grid))

!

Hl\_update=0d0

do i=1,grid

if (i.eq.1) then

Hl\_update(i)=Hl(i)+D\*dt/dz/dz\*( Hl(i)-2\*Hl(i)+Hl(i+1))

else if (i.eq.grid) then

Hl\_update(i)=Hs

!Hl\_update(i)=Hl(i)+D\*dt/dz/dz\*( Hl(i)-2\*Hl(i)+Hs )

else

Hl\_update(i)=Hl(i)+D\*dt/dz/dz\*( Hl(i-1)-2\*Hl(i)+Hl(i+1) )

endif

enddo

do i=1,grid

Hl(i)=Hl\_update(i)

enddo

deallocate(Hl\_update)

end subroutine FDM

!-------------------------------------------------------------------------------------

subroutine FDM\_s(Hl,Hs,D,dz,dt,z,grid)

implicit none

integer :: i, grid

real(8), allocatable, dimension(:) :: Hl, z, Hl\_update

real(8) :: Hs,D,dz,dt

! Allocate temp array

allocate(Hl\_update(grid))

!

Hl\_update=0d0

do i=1,grid

if (i.eq.1) then

Hl\_update(i)=Hl(i)+D\*dt/dz/dz\*( Hl(i)-2\*Hl(i)+Hl(i+1) )+D\*dt/dz/z(i)\*( Hl(i+1)-Hl(i))

else if (i.eq.grid) then

Hl\_update(i)=Hs

!Hl\_update(i)=Hl(i)+D\*dt/dz/dz\*( Hl(i)-2\*Hl(i)+Hs )+D\*dt/dz/z(i)\*( Hs-Hl(i))

else

Hl\_update(i)=Hl(i)+D\*dt/dz/dz\*( Hl(i-1)-2\*Hl(i)+Hl(i+1) )+D\*dt/dz/z(i)\*( Hl(i+1)-Hl(i) )

endif

enddo

do i=1,grid

Hl(i)=Hl\_update(i)

enddo

deallocate(Hl\_update)

end subroutine FDM\_s

!-------------------------------------------------------------------------------------

subroutine local\_eq(Hl,Ht,Nl,Nt,k,T)

implicit none

real(8) :: Hl,Ht,Nl,Nt,Eb,k,T

real(8) :: y1,y2,y3,gl,gt,total

!

total=Hl+Ht

if (total<=1e-20) return!goto 60 !.le.

gl=Hl/Nl

gt=Ht/Nt

y1=Nt

y2=-1\*(total+Nl/k+Nt)

y3=total

gt=(-y2-dsqrt(y2\*\*2-4\*y1\*y3))/2/y1

Ht=gt\*Nt

Hl=total-Ht

if ((total-Ht)<=1e-20) Hl=0.0 !.le.

60 end subroutine local\_eq

!-------------------------------------------------------------------------------------

subroutine kinetic(Hl,Ht,Nl,Nt,Q,Eb,dt,T)

implicit none

real(8) :: Hl,Nl,Ht,Nt,Q,Eb,dt,T

real(8) :: Ht\_up,Hl\_up, Ptl, Plt

real(8) :: prob

!

50 Plt=prob(Nt,Nl,Ht,Hl,Q,T,dt)

Ptl=prob(Nl,Nt,Hl,Ht,Eb+Q,T,dt)

Hl\_up=Ht\*Ptl+Hl\*(1-Plt)

Ht\_up=Hl\*Plt+Ht\*(1-Ptl)

if (Ht\_up<0 .or. Ht\_up>Nt) then

dt=dt/2

print \*, 'Too large dt (kinetic)'

write(4,'(F9.2,E11.4,a)') T-273,dt,' 2'

goto 50

endif

Hl=Hl\_up

Ht=Ht\_up

end subroutine kinetic

!-------------------------------------------------------------------------------------

real(8) function prob(Nt,Nl,Ht,Hl,Q,T,dt)

implicit none

real(8) :: Nt,Nl,Ht,Hl,Q,k,T,dt

real(8), parameter :: R=8.3144621d0 !Gas constant J/mol

real(8), parameter :: Mu=1d13 !Prefactor

!

k=exp(-Q/R/T)

prob=k\*(Nt-Ht)/(Nt+Nl-(Ht+Hl))

prob=1-(1-prob)\*\*(Mu\*dt)

return

end function prob

!-------------------------------------------------------------------------------------