%%% Values of Constants Used in the NaAlH4 Model

Pref 101325[Pa]

Uref 0.1[m/s]

Lref 0.1[m]

Cref Pref/(R\*Tref)[mole/m^3]

Tref 300[K]

rho\_ref M\_H2\*Cref[kg/m^3]

C0 P0/(R\*T0)[mole/m^3]

Dp 3e-7[m]

epsilon 0.5

M\_NaAlH4 54/1000[kg/mole]

M\_H2 2.016/1000[kg/mole]

R 8.314[J/(mole\*K)]

P0 101325[Pa]

T0 373[K]

Tinj 373[K]

Vinj 14[m/s]

Dinj 0.0127[m]

Cout C0

rho\_cool 820[kg/m^3]

k\_cool 0.325[W/(m\*K)]

Cp\_cool 820[J/(kg\*K)]

mu\_cool 3e-3[Pa\*s]

D\_cool 0.0168[m/s]

Vcool 13.0[m/s]

T\_cool 373[K]

h\_contact\_tube 5.56e-4[W/m^2\*K]

H\_contact\_bed 1e-6[W/m^2\*K]

rho\_bed 720.0[kg/m^3]

k\_bed 0.325[W/(m\*K)]

Cp\_bed 820[J/(kg\*K)]

S0 4.48e6[W/m^3]

tau 60[s]

a -log(0.1)/tau

A1F 1e8

E1F 80[kJ/mole]

A1B 4e12

E1B 110[kJ/mole]

Chi1 2

A2F 1.5e5

E2F 70[kJ/mole]

A2B 6e12

E2B 110[kJ/mole]

Chi2 1

DHR1 -4475

DSR1 -14.83

DHR2 -6150

DSR2 -16.22

DH\_rx1 37000[J/mole]

Dh\_rx2 47000[J/mole]

C10 0[mole/m^3]

C20 0[mole/m^3]

C30 13333.33[mole/m^3]

%%% Global Expressions Used in NaAlH4 Model

mu\_H2 5.1899\*10^-8\*TK-1.23594\*10^-10\*TK^2+2.06597\*10^-13\*TK^3-1.30208\*10^-16\*TK^4[

rho\_H2 C\*M\_H2

rho\_H2\_nd rho\_H2/rho\_ref

k\_H2 (0.7042\*TK-1.470\*10^-4\*TK^2-3.652\*10^-7\*TK^3-1.738\*10^-10\*TK^4)/1000

Cp\_H2 5.1899\*10^-8\*TK-1.23594\*10^-10\*TK^2+2.06597\*10^-13\*TK^3-1.30208\*10^-16\*TK^4

Pinj 49\*P0\*(1-exp(-.456\*t))+P0

G\_H2\_inj (Cinj\*M\_H2)\*Vinj

G\_cool rho\_cool\*Vcool

Pr\_H2 visc\_H2(Tinj)\*spec\_heat\_H2(Tinj)/therm\_cond\_H2(Tinj)

Pr\_cool mu\_cool\*Cp\_cool/k\_cool

h\_conv\_H2 0.023\*therm\_cond\_H2(Tinj)/Dinj\*(G\_H2\_inj\*Dinj/visc\_H2(Tinj))^0.8\*Pr\_H2^0.4

h\_conv\_cool 0.023\*k\_cool/D\_cool\*(G\_cool\*D\_cool/mu\_cool)^0.8\*Pr^0.4

TK T\_nd\*Tref

T TK

%%% Subdomain Expressions Used in the NaAlH4 Model

P C\*R\*TK

u\_nd -Dp^2\*Pref\*(epsilon/(1-epsilon))^2\*diff(Pnd,x)/(150\*mu\_H2\*Uref)

v\_nd -Dp^2\*Pref\*(epsilon/(1-epsilon))^2\*diff(Pnd,y)/(150\*mu\_H2\*Uref)

w\_nd -Dp^2\*Pref\*(epsilon/(1-epsilon))^2\*diff(Pnd,z)/(150\*mu\_H2\*Uref)

Source C1t\*DH\_rx1-0.5\*C3t\*DH\_rx\_2

P\_nd P/Pref

u u\_nd\*Uref

v v\_nd\*Uref

w w\_nd\*Uref

Peq1 100000\*exp(DHR1/TK-DSR1)

Peq2 100000\*exp(DHR2/TK-DSR2)

C2sat 0

C3sat 1-125\*wf(TK)/7

C2 C20-(C11-C10+C3-C30)/3

Ceqv C10+3\*C20+C30

r1F A1F\*Ceqv\*exp(-1000\*E1F/(R\*TK))\*(P-Peq1)\*(3\*C2/Ceqv-C2sat)^Chi1/Peq1

r1B -A1B\*Ceqv\*exp(-1000\*E1B/(R\*TK))\*(Peq1-P)\*(C11/Ceqv)^Chi1/Peq1

r2F -A2F\*Ceqv\*exp(-1000\*E2F/(R\*TK))\*(P-Peq2)\*(C3/Ceqv-C3sat)^Chi2/Peq2

r2B A2B\*Ceqv\*exp(-1000\*E2B/(R\*TK))\*(Peq2-P)\*(3\*C2/Ceqv)^Chi2/Peq2

C C\_nd\*Cref

C11 C1\*(C1>0)