

Appendix E
User-defined Function

**User-defined Function
For Homogenous model**

```
#include "udf.h"
DEFINE_PROPERTY(Keffvf1_Al2O3,c,t)
{
    real kf,kp,klr,keff;
    real h,a,vf,con;
    real beto,betl,gam;
    real temp = C_T(c,t);
    kf=0.613;
    kp=40;
    vf=0.01;
    con=30;
    a=6.5;
    h=0.01*(temp-273)*pow(a,0.35);
    klr=con*h*kf/a;
    gam=h/a;
    beto=1+gam;
    betl=1+(gam/2);
    keff=(((kp-klr)*vf*klr*((2*pow(betl,3))-
pow(beto,3)+1))+((kp+(2*klr))*pow(betl,3)*((vf*pow(beto,3)*(klr-
kf))+kf)))/(((pow(betl,3)*(kp+(2*klr)))-((kp-klr)*vf*(pow(betl,3)+pow(beto,3)-1))));

    return keff;
}

DEFINE_PROPERTY(Keffvf2p5_Al2O3,c,t)
{

    real kf,kp,klr,keff;
    real h,a,vf,con;
    real beto,betl,gam;
```

```

    real temp = C_T(c,t);
    kf=0.613;
    kp=40;
    vf=0.025;
    con=30;
    a=6.5;
    h=0.01*(temp-273)*pow(a,0.35);
    klr=con*h*kf/a;
    gam=h/a;
    beto=1+gam;
    betl=1+(gam/2);
    keff=(((kp-klr)*vf*klr*((2*pow(betl,3))-
pow(beto,3)+1))+((kp+(2*klr))*pow(betl,3)*(((vf*pow(beto,3)*(klr-
kf))+kf)))/(((pow(betl,3)*(kp+(2*klr)))-((kp-klr)*vf*(pow(betl,3)+pow(beto,3)-1)))));

    return keff;
}

DEFINE_PROPERTY(Keffvf5_Al2O3,c,t)
{
    real kf,kp,klr,keff;
    real h,a,vf,con;
    real beto,betl,gam;
    real temp = C_T(c,t);
    kf=0.613;
    kp=40;
    vf=0.05;
    con=30;
    a=6.5;
    h=0.01*(temp-273)*pow(a,0.35);
    klr=con*h*kf/a;
    gam=h/a;
    beto=1+gam;
    betl=1+(gam/2);

```

```

    keff=(((kp-klr)*vf*klr*((2*pow(betl,3))-
pow(beto,3)+1))+((kp+(2*klr))*pow(betl,3)*((vf*pow(beto,3)*(klr-
kf))+kf)))/(((pow(betl,3)*(kp+(2*klr)))-((kp-klr)*vf*(pow(betl,3)+pow(beto,3)-1))));

```

```

    return keff;
}

```

```

DEFINE_PROPERTY(Keffvf7p5_Al2O3,c,t)

```

```

{
    real kf,kp,klr,keff;
    real h,a,vf,con;
    real beto,betl,gam;
    real temp = C_T(c,t);
    kf=0.613;
    kp=40;
    vf=0.075;
    con=30;
    a=6.5;
    h=0.01*(temp-273)*pow(a,0.35);
    klr=con*h*kf/a;
    gam=h/a;
    beto=1+gam;
    betl=1+(gam/2);
    keff=(((kp-klr)*vf*klr*((2*pow(betl,3))-
pow(beto,3)+1))+((kp+(2*klr))*pow(betl,3)*((vf*pow(beto,3)*(klr-
kf))+kf)))/(((pow(betl,3)*(kp+(2*klr)))-((kp-klr)*vf*(pow(betl,3)+pow(beto,3)-1))));

    return keff;
}

```

```

DEFINE_PROPERTY(Keffvf10_Al2O3,c,t)

```

```

{
    real kf,kp,klr,keff;
    real h,a,vf,con;

```

```

real beto,betl,gam;
real temp = C_T(c,t);
kf=0.613;
kp=40;
vf=0.1;
con=30;
a=6.5;
h=0.01*(temp-273)*pow(a,0.35);
klr=con*h*kf/a;
gam=h/a;
beto=1+gam;
betl=1+(gam/2);
keff=(((kp-klr)*vf*klr*((2*pow(betl,3))-
pow(beto,3)+1))+((kp+(2*klr))*pow(betl,3)*(((vf*pow(beto,3)*(klr-
kf))+kf)))/(((pow(betl,3)*(kp+(2*klr)))-((kp-klr)*vf*(pow(betl,3)+pow(beto,3)-1)))));

return keff;
}

DEFINE_PROPERTY(Keffvf1_CuO,c,t)
{
real kf,kp,klr,keff;
real h,a,vf,con;
real beto,betl,gam;
real temp = C_T(c,t);
kf=0.613;
kp=40;
vf=0.01;
con=110;
a=6.5;
h=0.01*(temp-273)*pow(a,0.35);
klr=con*h*kf/a;
gam=h/a;
beto=1+gam;

```

```

    betl=1+(gam/2);
    keff=((((kp-klr)*vf*klr*((2*pow(betl,3))-
pow(beto,3)+1))+((kp+(2*klr))*pow(betl,3)*((vf*pow(beto,3)*(klr-
kf))+kf)))/(((pow(betl,3)*(kp+(2*klr)))-((kp-klr)*vf*(pow(betl,3)+pow(beto,3)-1))));

    return keff;
}

```

```

DEFINE_PROPERTY(Keffvf2p5_CuO,c,t)

```

```

{
    real kf,kp,klr,keff;
    real h,a,vf,con;
    real beto,betl,gam;
    real temp = C_T(c,t);
    kf=0.613;
    kp=40;
    vf=0.025;
    con=110;
    a=6.5;
    h=0.01*(temp-273)*pow(a,0.35);
    klr=con*h*kf/a;
    gam=h/a;
    beto=1+gam;
    betl=1+(gam/2);
    keff=((((kp-klr)*vf*klr*((2*pow(betl,3))-
pow(beto,3)+1))+((kp+(2*klr))*pow(betl,3)*((vf*pow(beto,3)*(klr-
kf))+kf)))/(((pow(betl,3)*(kp+(2*klr)))-((kp-klr)*vf*(pow(betl,3)+pow(beto,3)-1))));

    return keff;
}

```

```

DEFINE_PROPERTY(Keffvf5_CuO,c,t)

```

```

{
    real kf,kp,klr,keff;

```

```

real h,a,vf,con;
real beto,betl,gam;
real temp = C_T(c,t);
kf=0.613;
kp=40;
vf=0.05;
con=110;
a=6.5;
h=0.01*(temp-273)*pow(a,0.35);
klr=con*h*kf/a;
gam=h/a;
beto=1+gam;
betl=1+(gam/2);
keff=(((kp-klr)*vf*klr*((2*pow(betl,3))-
pow(beto,3)+1))+((kp+(2*klr))*pow(betl,3)*((vf*pow(beto,3)*(klr-
kf))+kf)))/(((pow(betl,3)*(kp+(2*klr)))-((kp-klr)*vf*(pow(betl,3)+pow(beto,3)-1))));

return keff;
}

DEFINE_PROPERTY(Keffvf7p5_CuO,c,t)
{
real kf,kp,klr,keff;
real h,a,vf,con;
real beto,betl,gam;
real temp = C_T(c,t);
kf=0.613;
kp=40;
vf=0.075;
con=110;
a=6.5;
h=0.01*(temp-273)*pow(a,0.35);
klr=con*h*kf/a;
gam=h/a;

```

```

    beto=1+gam;
    betl=1+(gam/2);
    keff=(((kp-klr)*vf*klr*((2*pow(betl,3))-
pow(beto,3)+1))+((kp+(2*klr))*pow(betl,3)*((vf*pow(beto,3)*(klr-
kf))+kf)))/(((pow(betl,3)*(kp+(2*klr)))-((kp-klr)*vf*(pow(betl,3)+pow(beto,3)-1))));

    return keff;
}
DEFINE_PROPERTY(Keffvf10_CuO,c,t)
{
    real kf,kp,klr,keff;
    real h,a,vf,con;
    real beto,betl,gam;
    real temp = C_T(c,t);
    kf=0.613;
    kp=40;
    vf=0.1;
    con=110;
    a=6.5;
    h=0.01*(temp-273)*pow(a,0.35);
    klr=con*h*kf/a;
    gam=h/a;
    beto=1+gam;
    betl=1+(gam/2);
    keff=(((kp-klr)*vf*klr*((2*pow(betl,3))-
pow(beto,3)+1))+((kp+(2*klr))*pow(betl,3)*((vf*pow(beto,3)*(klr-
kf))+kf)))/(((pow(betl,3)*(kp+(2*klr)))-((kp-klr)*vf*(pow(betl,3)+pow(beto,3)-1))));

    return keff;
}

```

For Species model

```
#include "udf.h"
```

```
DEFINE_PROPERTY(Keff_Al2O3,c,t)
```

```

{
    real kf,kp,klr,keff,pp,pw;
    real h,a,vf,con;
    real beto,betl,gam;
    real temp = C_T(c,t);
    int i=0;
    real mf = C_YI(c,t,i);
    kf=0.613;
    kp=40;
    con=30;
    a=6.5;
    pp=3970;
    pw=998.2;
    vf=((mf/pp)/((1/pw)+(mf/pp)-(mf/pw)));
    h=0.01*(temp-273)*pow(a,0.35);
    klr=con*h*kf/a;
    gam=h/a;
    beto=1+gam;
    betl=1+(gam/2);
    keff=(((kp-klr)*vf*klr*((2*pow(betl,3))-
pow(beto,3)+1))+((kp+(2*klr))*pow(betl,3)*((vf*pow(beto,3)*(klr-
kf))+kf)))/(((pow(betl,3)*(kp+(2*klr)))-((kp-klr)*vf*(pow(betl,3)+pow(beto,3)-1))));

    return keff;
}

```

```

DEFINE_PROPERTY(Keff_CuO,c,t)

```

```

{
    real kf,kp,klr,keff,pp,pw;
    real h,a,vf,con;
    real beto,betl,gam;
    real temp = C_T(c,t);
    int i=0;
    real mf = C_YI(c,t,i);

```

```

kf=0.613;
kp=40;
con=110;
a=6.5;
pp=6300;
pw=998.2;
vf=((mf/pp)/((1/pw)+(mf/pp)-(mf/pw)));
h=0.01*(temp-273)*pow(a,0.35);
klr=con*h*kf/a;
gam=h/a;
beto=1+gam;
betl=1+(gam/2);
keff=((((kp-klr)*vf*klr*((2*pow(betl,3))-
pow(beto,3)+1))+((kp+(2*klr))*pow(betl,3)*((vf*pow(beto,3)*(klr-
kf))+kf)))/(((pow(betl,3)*(kp+(2*klr)))-((kp-klr)*vf*(pow(betl,3)+pow(beto,3)-1))));

return keff;
}

```