POLITECNICO DI TORINO

DOCTORATE SCHOOL
Ph.D. in Metrology: Measuring science and Technique – XXVI doctoral cycle

PhD Thesis

Process Intensification Vs. Reliability

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%Heat transfer along solid
dTs(i)=(K2/(rs2*cps2*Dz))*((-Ts(i)+Ts(i+1))/Dz)-((h2*av2)/(rs2*cps2*(1-eps2)))*(Ts(i)↙
-Tg(i))-((DHr*ru2*eps2)/(rs2*cps2*(1-eps2)))*((Dx)/Dz);
%
%Along layer of catalyst
%
for i=33:45
    %Heat gas balance
    Tg(i)=(((h2*av2*Dz)/(ru2*cpg*eps2))*Ts(i)+Tg(i-1))/(((h2*av2*Dz)/(ru2*cpg*eps2))↙
+1);
    if sint(i)>0 %If the catalyst in this section is sintered not occur the chemical↙
reaction
        dx(i)=((x(i-1)-x(i))/Dz)*(u2*Tg(i));
        do(i)=((o(i-1)-o(i))/Dz)*(u2*Tg(i));
        Dx=0;
    else
        if x(i-1)>0 && o(i-1)>0 %Is present all reagent
            if Ts(i)>=Tre %Temperature is higher than reaction temperature
               if o(i-1)/(PMO*2.5)>x(i-1)/PMC %Excess of oxygen
                   x(i)=0;
                   do(i)=(((o(i-1)-((x(i-1)/PMC)*(PMO*2.5)))-o(i))/Dz)*(u2*Tg(i));
                   Dx=x(i)-x(i-1);
               else %Excess of VOCs
                   o(i)=0;
                   dx(i)=(((x(i-1)-((o(i-1)*PMC)/(PMO*2.5)))-x(i))/Dz)*(u2*Tg(i));
                   Dx=(o(i)-o(i-1))/(PMO*2.5)*PMC;
               end
            else %Temperature is Lower than reaction temperature
                dx(i)=((x(i-1)-x(i))/Dz)*(u2*Tg(i));
                do(i)=((o(i-1)-o(i))/Dz)*(u2*Tg(i));
                Dx=0;
            end
        else
            if x(i-1)<=0 %if in gas is not present VOCs, Oxygen move a long reactor
                x(i)=0;
                do(i)=((o(i-1)-o(i))/Dz)*(u2*Tg(i));
            end
            if o(i-1)<=0 %if in gas is not present Oxygen, VOCs move a long reactor
                o(i)=0;
                dx(i)=((x(i-1)-x(i))/Dz)*(u2*Tg(i));
            end
            Dx=0;
        end
    end
    if x(i)<0 %concentration below zero is impossible
        x(i)=0;
    end
    if o(i)<0 %concentration below zero is impossible
        o(i)=0;
    end
    %Heat transfer along solid
    dTs(i)=(K2/(rs2*cps2*Dz))*((Ts(i+1)-2*Ts(i)+Ts(i-1))/Dz)-((h2*av2)/(rs2*cps2*(1-↙
eps2)))*(Ts(i)-Tg(i))-(((DHr*ru2*eps2)/(rs2*cps2*(1-eps2)))*((Dx)/Dz));
end
%
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%Interface catalyst-inert (side catalyst)
i=46;
%Heat gas balance
Tg(i)=(((h2*av2*Dz)/(ru2*cpg))*Ts(i)+Tg(i-1))/(((h2*av2*Dz)/(ru2*cpg))+1);
if sint(i)>0 %If the catalyst in this section is sintered not occur the chemical↙
reaction
    dx(i)=((x(i-1)-x(i))/Dz)*(u2*Tg(i));
    do(i)=((o(i-1)-o(i))/Dz)*(u2*Tg(i));
    Dx=0;
else
    if x(i-1)>0 && o(i-1)>0 %Is present all reagent
        if Ts(i)>=Tre %Temperature is higher than reaction temperature
            if o(i-1)/(PMO*2.5)>x(i-1)/PMC %Excess of oxygen
                x(i)=0;
                do(i)=(((o(i-1)-((x(i-1)/PMC)*(PMO*2.5)))-o(i))/Dz)*(u2*Tg(i));
                Dx=x(i)-x(i-1);
            else %Excess of VOCs
                o(i)=0;
                dx(i)=(((x(i-1)-((o(i-1)*PMC)/(PMO*2.5)))-x(i))/Dz)*(u2*Tg(i));
                Dx=(o(i)-o(i-1))/(PMO*2.5)*PMC;
            end
        else %Temperature is Lower than reaction temperature
            dx(i)=((x(i-1)-x(i))/Dz)*(u2*Tg(i));
            do(i)=((o(i-1)-o(i))/Dz)*(u2*Tg(i));
            Dx=0;
        end
    else
        if x(i-1)<=0 %if in gas is not present VOCs, Oxygen move a long reactor
            x(i)=0;
            do(i)=((o(i-1)-o(i))/Dz)*(u2*Tg(i));
        end
        if o(i-1)<=0 %if in gas is not present Oxygen, VOCs move a long reactor
            o(i)=0;
            dx(i)=((x(i-1)-x(i))/Dz)*(u2*Tg(i));
        end
        Dx=0;
    end
end
if x(i)<0 %concentration below zero is impossible
    x(i)=0;
end
if o(i)<0 %concentration below zero is impossible
    o(i)=0;
end
%Heat transfer along solid
dTs(i)=(K2/(rs2*cps2*Dz))*((-Ts(i)+Ts(i-1))/Dz)-((h2*av2)/(rs2*cps2*(1-eps2)))*(Ts(i)↙
-Tg(i))+(K1/(rs2*cps2*Dz))*((-Ts(i)+Ts(i+1))/Dz)-(((DHr*ru2*eps2)/(rs2*cps2*(1-↙
eps2)))*((Dx)/Dz));
%
%Interface catalyst-inert (side inert)
i=47;
%Heat gas balance
Tg(i)=(((h1*av1*Dz)/(ru1*cpg*eps1))*Ts(i)+Tg(i-1))/(((h1*av1*Dz)/(ru1*cpg*eps1))+1);
%Mass balance for component
dx(i)=((x(i-1)-x(i))/Dz)*(u1*Tg(i));
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do(i)=((o(i-1)-o(i))/Dz)*(u1*Tg(i));
if x(i)<0 %concentration below zero is impossible
    x(i)=0;
end
if o(i)<0 %concentration below zero is impossible
    o(i)=0;
end
%Heat transfer along solid
dTs(i)=(K2/(rs1*cps1*Dz))*((-Ts(i)+Ts(i-1))/Dz)-((h1*av1)/(rs1*cps1*(1-eps1)))*(Ts(i)
-Tg(i))+(K1/(rs1*cps1*Dz))*((Ts(i-1)-Ts(i))/Dz);
%
%Along layer of solid inert
for i=48:60
    %Heat gas balance
    Tg(i)=(((h1*av1*Dz)/(ru1*cpg*eps1))*Ts(i)+Tg(i-1))/(((h1*av1*Dz)/(ru1*cpg*eps1))
+1);
    %Mass balance for component
    dx(i)=((x(i-1)-x(i))/Dz)*(u1*Tg(i));
    do(i)=((o(i-1)-o(i))/Dz)*(u1*Tg(i));
    if x(i)<0 %concentration below zero is impossible
        x(i)=0;
    end
    if o(i)<0 %concentration below zero is impossible
        o(i)=0;
    end
    %Heat transfer along solid
    dTs(i)=(K1/(rs1*cps1*Dz))*((Ts(i+1)-2*Ts(i)+Ts(i-1))/Dz)-((h1*av1)/(rs1*cps1*(1-
eps1)))*(Ts(i)-Tg(i));
end
%
%Last section of reactor
i=ns;
%Heat gas balance
Tg(i)=(((h1*av1*Dz)/(ru1*cpg*eps1))*Ts(i)+Tg(i-1))/(((h1*av1*Dz)/(ru1*cpg*eps1))+1);
%Mass balance for component
dx(i)=((x(i-1)-x(i))/Dz)*(u1*Tg(i));
do(i)=((o(i-1)-o(i))/Dz)*(u1*Tg(i));
if x(i)<0 %concentration below zero is impossible
    x(i)=0;
end
 if o(i)<0 %concentration below zero is impossible
    o(i)=0;
 end
%Heat transfer along solid
dTs(i)=(K1/(rs1*cps1*Dz))*((-Ts(i)+Ts(i-1))/Dz)-((h1*av1)/(rs1*cps1*(1-eps1)))*(Ts(i)
-Tg(i));
%Up date derivate vector
for i=1:ns
    fy(i)=dTs(i);
    fy(i+ns)=dx(i);
    fy(i+2*ns)=do(i);
end
```

```
function fy=m2(t,y)
global cpg Ting ns av1 av2 eps1 eps2 K1 K2 DHr rs1 rs2 cps1 cps2 xin Tre h1
global h2 S ru1 ru2 ru3 Dz u1 u2 u3 PMC PMO oin Tg Qre sint
%
%Reactor in emergency
fy=zeros(3*ns,1);
for i=1:ns
    Ts(i)=y(i);      %Solid Temperature
    Tg(i)=Tg(i);     %Gas temperature
    x(i)=y(i+ns);    %VOCs concentration
    o(i)=y(i+2*ns); %Oxygen concentration
end
%
%Gas input zone, reactor center
i=31;
%Heat gas balance
Tg(i)=Ting+(Qre/(ru3*cpg*S));
%Mass balance for component
dx(i)=((xin-x(i))/Dz)*(u3*Tg(i));
do(i)=((oin-o(i))/Dz)*(u3*Tg(i));
if x(i)<0 %concentration below zero is impossible
    x(i)=0;
end
if o(i)<0 %concentration below zero is impossible
    o(i)=0;
end
%In this section is not present solid
%
%First half of the reatttore
%
%Reverse order of the indexes
for i=1:31
    Ts1(i)=Ts(32-i);     %Solid Temperature
    Tg1(i)=Tg(32-i);     %Gas temperature
    x1(i)=x(32-i);       %VOCs concentration
    o1(i)=o(32-i);       %Oxygen concentration
end
%
%Interface heater-catalyst (side catalyst)
i=2;
%Heat gas balance
Tg1(i)=(((h2*av2*Dz)/(ru2/2*cpg*eps2))*Ts1(i)+Tg1(i-1))/(((h2*av2*Dz)/↙
(ru2/2*cpg*eps2))+1);
if sint(i)>0 %If the catalyst in this section is sintered not occur the chemical↙
reaction
    dx1(i)=((x1(i-1)-x1(i))/Dz)*(u2*Tg1(i)/2);
    do1(i)=((o1(i-1)-o1(i))/Dz)*(u2*Tg1(i)/2);
    Dx=0;
else
    if x1(i-1)>0 && o1(i-1)>0 %Is present all reagent
        if Ts1(i)>=Tre %Temperature is higher than reaction temperature
            if o1(i-1)/(PMO*2.5)>x1(i-1)/PMC %Excess of oxygen
                x1(i)=0;
                do1(i)=(((o1(i-1)-((x1(i-1)/PMC)*(PMO*2.5)))-o1(i))/Dz)*(u2*Tg1(i)↙
/2);
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```
                Dx=x1(i)-x1(i-1);
            else  %Excess of VOCs
                o1(i)=0;
                dx1(i)=(((x1(i-1)-((o1(i-1)*PMC)/(PMO*2.5)))-x1(i))/Dz)*(u2*Tg1(i)↙
/2);
                Dx=(o1(i)-o1(i-1))/(PMO*2.5)*PMC;
            end
        else %Temperature is Lower than reaction temperature
            dx1(i)=((x1(i-1)-x1(i))/Dz)*(u2*Tg1(i)/2);
            do1(i)=((o1(i-1)-o1(i))/Dz)*(u2*Tg1(i)/2);
            Dx=0;
        end
    else
        if x1(i-1)<=0 %if in gas is not present VOCs, Oxygen move a long reactor
            x1(i)=0;
            do1(i)=((o1(i-1)-o1(i))/Dz)*(u2*Tg1(i)/2);
        end
        if o1(i-1)<=0 %if in gas is not present Oxygen, VOCs move a long reactor
            o1(i)=0;
            dx1(i)=((x1(i-1)-x1(i))/Dz)*(u2*Tg1(i)/2);
        end
        Dx=0;
    end
end
if x1(i)<0 %concentration below zero is impossible
    x1(i)=0;
end
if o1(i)<0 %concentration below zero is impossible
    o1(i)=0;
end
%Heat transfer along solid
dTs1(i)=(K2/(rs2*cps2*Dz))*((-Ts1(i)+Ts1(i+1))/Dz)-((h2*av2)/(rs2*cps2*(1-eps2)))*↙
(Ts1(i)-Tg1(i))-((DHr*ru2/2*eps2)/(rs2*cps2*(1-eps2)))*((Dx)/Dz);
%
%Along layer of catalyst
%
for i=3:15
    %Heat gas balance
    Tg1(i)=(((h2*av2*Dz)/(ru2/2*cpg*eps2))*Ts1(i)+Tg1(i-1))/(((h2*av2*Dz)/↙
(ru2/2*cpg*eps2))+1);
    if sint(i)>0 %If the catalyst in this section is sintered not occur the chemical↙
reaction
        dx1(i)=((x1(i-1)-x1(i))/Dz)*(u2/2*Tg1(i));
        do1(i)=((o1(i-1)-o1(i))/Dz)*(u2/2*Tg1(i));
        Dx=0;
    else
        if x1(i-1)>0 && o1(i-1)>0 %Is present all reagent
            if Ts1(i)>=Tre %Temperature is higher than reaction temperature
                if o1(i-1)/(PMO*2.5)>x1(i-1)/PMC %Excess of oxygen
                    x1(i)=0;
                    do1(i)=(((o1(i-1)-((x1(i-1)/PMC)*(PMO*2.5)))-o1(i))/Dz)*(u2*Tg1↙
(i)/2);
                    Dx=x1(i)-x1(i-1);
                else %Excess of VOCs
                    o1(i)=0;
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```
                    dx1(i)=(((x1(i-1)-((o1(i-1)*PMC)/(PMO*2.5)))-x1(i))/Dz)*(u2*Tg1↙
(i)/2);
                    Dx=(o1(i)-o1(i-1))/(PMO*2.5)*PMC;
                end
            else %Temperature is Lower than reaction temperature
                dx1(i)=((x1(i-1)-x1(i))/Dz)*(u2*Tg1(i)/2);
                do1(i)=((o1(i-1)-o1(i))/Dz)*(u2*Tg1(i)/2);
                Dx=0;
            end
        else
            if x1(i-1)<=0 %if in gas is not present VOCs, Oxygen move a long reactor
                x1(i)=0;
                do1(i)=((o1(i-1)-o1(i))/Dz)*(u2*Tg1(i)/2);
            end
          if o1(i-1)<=0 %if in gas is not present Oxygen, VOCs move a long reactor
                o1(i)=0;
                dx1(i)=((x1(i-1)-x1(i))/Dz)*(u2*Tg1(i)/2);
          end
          Dx=0;
        end
    end
    if x1(i)<0 %concentration below zero is impossible
        x1(i)=0;
    end
    if o1(i)<0 %concentration below zero is impossible
        o1(i)=0;
    end
    %Heat transfer along solid
    dTs1(i)=(K2/(rs2*cps2*Dz))*((Ts1(i+1)-2*Ts1(i)+Ts1(i-1))/Dz)-((h2*av2)/(rs2*cps2*↙
(1-eps2)))*(Ts1(i)-Tg1(i))-(((DHr*ru2/2*eps2)/(rs2*cps2*(1-eps2)))*((Dx)/Dz));
end
%
%Interface catalyst-inert (side catalyst)
i=16;
%Heat gas balance
Tg1(i)=(((h2*av2*Dz)/(ru2/2*cpg))*Ts1(i)+Tg1(i-1))/(((h2*av2*Dz)/(ru2/2*cpg))+1);
if sint(i)>0 %If the catalyst in this section is sintered not occur the chemical↙
reaction
    dx1(i)=((x1(i-1)-x1(i))/Dz)*(u2/2*Tg1(i));
    do1(i)=((o1(i-1)-o1(i))/Dz)*(u2/2*Tg1(i));
    Dx=0;
else
    if x1(i-1)>0 && o1(i-1)>0 %Is present all reagent
        if Ts1(i)>=Tre %Temperature is higher than reaction temperature
            if o1(i-1)/(PMO*2.5)>x1(i-1)/PMC %Excess of oxygen
                x1(i)=0;
                do1(i)=(((o1(i-1)-((x1(i-1)/PMC)*(PMO*2.5)))-o1(i))/Dz)*(u2*Tg1(i)↙
/2);
                Dx=x1(i)-x1(i-1);
            else %Excess of VOCs
                o1(i)=0;
                dx1(i)=(((x1(i-1)-((o1(i-1)*PMC)/(PMO*2.5)))-x1(i))/Dz)*(u2*Tg1(i)↙
/2);
                Dx=(o1(i)-o1(i-1))/(PMO*2.5)*PMC;
            end
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```
        else %Temperature is Lower than reaction temperature
            dx1(i)=((x1(i-1)-x1(i))/Dz)*(u2*Tg1(i)/2);
            do1(i)=((o1(i-1)-o1(i))/Dz)*(u2*Tg1(i)/2);
            Dx=0;
        end
    else
        if x1(i-1)<=0 %if in gas is not present VOCs, Oxygen move a long reactor
            x1(i)=0;
            do1(i)=((o1(i-1)-o1(i))/Dz)*(u2*Tg1(i)/2);
        end
        if o1(i-1)<=0 %if in gas is not present Oxygen, VOCs move a long reactor
            o1(i)=0;
            dx1(i)=((x1(i-1)-x1(i))/Dz)*(u2*Tg1(i)/2);
        end
        Dx=0;
    end
end
if x1(i)<0 %concentration below zero is impossible
    x1(i)=0;
end
if o1(i)<0 %concentration below zero is impossible
    o1(i)=0;
end
%Heat transfer along solid
dTs1(i)=(K2/(rs2*cps2*Dz))*((-Ts1(i)+Ts1(i-1))/Dz)-((h2*av2)/(rs2*cps2*(1-eps2)))*↙
(Ts1(i)-Tg1(i))+(K1/(rs2*cps2*Dz))*((-Ts1(i)+Ts1(i+1))/Dz);
%
%Interface catalyst-inert (side inert)
i=17;
%Heat gas balance
Tg1(i)=(((h1*av1*Dz)/(ru1/2*cpg*eps1))*Ts1(i)+Tg1(i-1))/(((h1*av1*Dz)/↙
(ru1/2*cpg*eps1))+1);
%Mass balance for component
dx1(i)=((x1(i-1)-x1(i))/Dz)*(u1*Tg1(i)/2);
do1(i)=((o1(i-1)-o1(i))/Dz)*(u1*Tg1(i)/2);
if x1(i)<0 %concentration below zero is impossible
    x1(i)=0;
end
if o1(i)<0 %concentration below zero is impossible
    o1(i)=0;
end
%Heat transfer along solid
dTs1(i)=(K2/(rs1*cps1*Dz))*((-Ts1(i)+Ts1(i-1))/Dz)-((h1*av1)/(rs1*cps1*(1-eps1)))*↙
(Ts1(i)-Tg1(i))+(K1/(rs1*cps1*Dz))*((Ts1(i-1)-Ts1(i))/Dz);
%
%Along layer of solid inert
for i=18:30
    %Heat gas balance
    Tg1(i)=(((h1*av1*Dz)/(ru1/2*cpg*eps1))*Ts1(i)+Tg1(i-1))/(((h1*av1*Dz)/↙
(ru1/2*cpg*eps1))+1);
    %Mass balance for component
    dx1(i)=((x1(i-1)-x1(i))/Dz)*(u1*Tg1(i)/2);
    do1(i)=((o1(i-1)-o1(i))/Dz)*(u1*Tg1(i)/2);
    if x1(i)<0 %concentration below zero is impossible
        x1(i)=0;
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    end
    if o1(i)<0 %concentration below zero is impossible
        o1(i)=0;
    end
    %Heat transfer along solid
    dTs1(i)=(K1/(rs1*cps1*Dz))*((Ts1(i+1)-2*Ts1(i)+Ts1(i-1))/Dz)-((h1*av1)/(rs1*cps1*↙
(1-eps1)))*(Ts1(i)-Tg1(i));
end
%
%Last section of reactor (first half)
i=31;
%Heat gas balance
Tg1(i)=(((h1*av1*Dz)/(ru1/2*cpg*eps1))*Ts1(i)+Tg1(i-1))/(((h1*av1*Dz)/↙
(ru1/2*cpg*eps1))+1);
%Mass balance for component
dx1(i)=((x1(i-1)-x1(i))/Dz)*(u1*Tg1(i)/2);
do1(i)=((o1(i-1)-o1(i))/Dz)*(u1*Tg1(i)/2);
if x1(i)<0 %concentration below zero is impossible
    x1(i)=0;
end
if o1(i)<0 %concentration below zero is impossible
    o1(i)=0;
end
%Heat transfer along solid
dTs1(i)=(K1/(rs1*cps1*Dz))*((-Ts1(i)+Ts1(i-1))/Dz)-((h1*av1)/(rs1*cps1*(1-eps1)))*↙
(Ts1(i)-Tg1(i));
%Reorder result
for i=1:30
    dTs(i)=dTs1(31-i+1);
    dx(i)=dx1(31-i+1);
    do(i)=do1(31-i+1);
    Ts(i)=Ts1(31-i+1);
    Tg(i)=Tg1(31-i+1);
    x(i)=x1(31-i+1);
    o(i)=o1(31-i+1);
end
%
%Second half of the reatttore
%
%Interface heater-catalyst (side catalyst)
i=32;
%Heat gas balance
Tg(i)=(((h2*av2*Dz)/(ru2/2*cpg*eps2))*Ts(i)+Tg(i-1))/(((h2*av2*Dz)/(ru2/2*cpg*eps2))↙
+1);
if sint(i)>0 %If the catalyst in this section is sintered not occur the chemical↙
reaction
    dx(i)=((x(i-1)-x(i))/Dz)*(u2*Tg(i)/2);
    do(i)=((o(i-1)-o(i))/Dz)*(u2*Tg(i)/2);
    Dx=0;
else
    if x(i-1)>0 && o(i-1)>0 %Is present all reagent
        if Ts(i)>=Tre %Temperature is higher than reaction temperature
            if o(i-1)/(PMO*2.5)>x(i-1)/PMC %Excess of oxygen
                x(i)=0;
                do(i)=(((o(i-1)-((x(i-1)/PMC)*(PMO*2.5)))-o(i))/Dz)*(u2*Tg(i)/2);
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                Dx=x(i)-x(i-1);
            else %Excess of VOCs
                o(i)=0;
                dx(i)=(((x(i-1)-((o(i-1)*PMC)/(PMO*2.5)))-x(i))/Dz)*(u2*Tg(i)/2);
                Dx=(o(i)-o(i-1))/(PMO*2.5)*PMC;
            end
        else %Temperature is Lower than reaction temperature
            dx(i)=((x(i-1)-x(i))/Dz)*(u2*Tg(i)/2);
            do(i)=((o(i-1)-o(i))/Dz)*(u2*Tg(i)/2);
            Dx=0;
        end
    else
        if x(i-1)<=0 %if in gas is not present VOCs, Oxygen move a long reactor
            x(i)=0;
            do(i)=((o(i-1)-o(i))/Dz)*(u2*Tg(i)/2);
        end
        if o(i-1)<=0 %if in gas is not present Oxygen, VOCs move a long reactor
            o(i)=0;
            dx(i)=((x(i-1)-x(i))/Dz)*(u2*Tg(i)/2);
        end
        Dx=0;
    end
end
if x(i)<0 %concentration below zero is impossible
    x(i)=0;
end
if o(i)<0 %concentration below zero is impossible
    o(i)=0;
end
%Heat transfer along solid
dTs(i)=(K2/(rs2*cps2*Dz))*((-Ts(i)+Ts(i+1))/Dz)-((h2*av2)/(rs2*cps2*(1-eps2)))*(Ts(i)↙
-Tg(i))-((DHr*ru2/2*eps2)/(rs2*cps2*(1-eps2)))*((Dx)/Dz);
%
%Along layer of catalyst
%
for i=33:45
    %Heat gas balance
    Tg(i)=(((h2*av2*Dz)/(ru2/2*cpg*eps2))*Ts(i)+Tg(i-1))/(((h2*av2*Dz)/↙
(ru2/2*cpg*eps2))+1);
    if sint(i)>0 %If the catalyst in this section is sintered not occur the chemical↙
reaction
        dx(i)=((x(i-1)-x(i))/Dz)*(u2/2*Tg(i));
        do(i)=((o(i-1)-o(i))/Dz)*(u2/2*Tg(i));
        Dx=0;
    else
        if x(i-1)>0 && o(i-1)>0 %Is present all reagent
            if Ts(i)>=Tre %Temperature is higher than reaction temperature
                if o(i-1)/(PMO*2.5)>x(i-1)/PMC %Excess of oxygen
                    x(i)=0;
                    do(i)=(((o(i-1)-((x(i-1)/PMC)*(PMO*2.5)))-o(i))/Dz)*(u2*Tg(i)/2);
                    Dx=x(i)-x(i-1);
                else %Excess of VOCs
                    o(i)=0;
                    dx(i)=(((x(i-1)-((o(i-1)*PMC)/(PMO*2.5)))-x(i))/Dz)*(u2*Tg(i)/2);
                    Dx=(o(i)-o(i-1))/(PMO*2.5)*PMC;
```

```
                end
            else %Temperature is Lower than reaction temperature
                dx(i)=((x(i-1)-x(i))/Dz)*(u2*Tg(i)/2);
                do(i)=((o(i-1)-o(i))/Dz)*(u2*Tg(i)/2);
                Dx=0;
            end
        else
            if x(i-1)<=0 %if in gas is not present VOCs, Oxygen move a long reactor
                x(i)=0;
                do(i)=((o(i-1)-o(i))/Dz)*(u2*Tg(i)/2);
            end
            if o(i-1)<=0 %if in gas is not present Oxygen, VOCs move a long reactor
                o(i)=0;
                dx(i)=((x(i-1)-x(i))/Dz)*(u2*Tg(i)/2);
            end
            Dx=0;
        end
    end
    if x(i)<0 %concentration below zero is impossible
        x(i)=0;
    end
    if o(i)<0 %concentration below zero is impossible
        o(i)=0;
    end
    %Heat transfer along solid
    dTs(i)=(K2/(rs2*cps2*Dz))*((Ts(i+1)-2*Ts(i)+Ts(i-1))/Dz)-((h2*av2)/(rs2*cps2*(1-↙
eps2)))*(Ts(i)-Tg(i))-(((DHr*ru2/2*eps2)/(rs2*cps2*(1-eps2)))*((Dx)/Dz));
end
%
%Interface catalyst-inert (side catalyst)
i=46;
%Heat gas balance
Tg(i)=(((h2*av2*Dz)/(ru2/2*cpg))*Ts(i)+Tg(i-1))/(((h2*av2*Dz)/(ru2/2*cpg))+1);
if sint(i)>0 %If the catalyst in this section is sintered not occur the chemical↙
reaction
    dx(i)=((x(i-1)-x(i))/Dz)*(u2/2*Tg(i));
    do(i)=((o(i-1)-o(i))/Dz)*(u2/2*Tg(i));
    Dx=0;
else
    if x(i-1)>0 && o(i-1)>0 %Is present all reagent
        if Ts(i)>=Tre %Temperature is higher than reaction temperature
            if o(i-1)/(PMO*2.5)>x(i-1)/PMC %Excess of oxygen
                x(i)=0;
                do(i)=(((o(i-1)-((x(i-1)/PMC)*(PMO*2.5)))-o(i))/Dz)*(u2*Tg(i)/2);
                Dx=x(i)-x(i-1);
            else %Excess of VOCs
                o(i)=0;
                dx(i)=(((x(i-1)-((o(i-1)*PMC)/(PMO*2.5)))-x(i))/Dz)*(u2*Tg(i)/2);
                Dx=(o(i)-o(i-1))/(PMO*2.5)*PMC;
            end
        else %Temperature is Lower than reaction temperature
            dx(i)=((x(i-1)-x(i))/Dz)*(u2*Tg(i)/2);
            do(i)=((o(i-1)-o(i))/Dz)*(u2*Tg(i)/2);
            Dx=0;
        end
```

```
    else
        if x(i-1)<=0 %if in gas is not present VOCs, Oxygen move a long reactor
            x(i)=0;
            do(i)=((o(i-1)-o(i))/Dz)*(u2*Tg(i)/2);
        end
        if o(i-1)<=0 %if in gas is not present Oxygen, VOCs move a long reactor
            o(i)=0;
            dx(i)=((x(i-1)-x(i))/Dz)*(u2*Tg(i)/2);
        end
        Dx=0;
    end
end
if x(i)<0 %concentration below zero is impossible
    x(i)=0;
end
if o(i)<0 %concentration below zero is impossible
    o(i)=0;
end
%Heat transfer along solid
dTs(i)=(K2/(rs2*cps2*Dz))*((-Ts(i)+Ts(i-1))/Dz)-((h2*av2)/(rs2*cps2*(1-eps2)))*(Ts(i)↙
-Tg(i))+(K1/(rs2*cps2*Dz))*((-Ts(i)+Ts(i+1))/Dz);
%
%Interface catalyst-inert (side inert)
i=47;
%Heat gas balance
Tg(i)=(((h1*av1*Dz)/(ru1/2*cpg*eps1))*Ts(i)+Tg(i-1))/(((h1*av1*Dz)/(ru1/2*cpg*eps1))↙
+1);
%Mass balance for component
dx(i)=((x(i-1)-x(i))/Dz)*(u1*Tg(i)/2);
do(i)=((o(i-1)-o(i))/Dz)*(u1*Tg(i)/2);
if x(i)<0 %concentration below zero is impossible
    x(i)=0;
end
if o(i)<0 %concentration below zero is impossible
    o(i)=0;
end
%Heat transfer along solid
dTs(i)=(K2/(rs1*cps1*Dz))*((-Ts(i)+Ts(i-1))/Dz)-((h1*av1)/(rs1*cps1*(1-eps1)))*(Ts(i)↙
-Tg(i))+(K1/(rs1*cps1*Dz))*((Ts(i-1)-Ts(i))/Dz);
%
%Along layer of solid inert
for i=48:60
    %Heat gas balance
    Tg(i)=(((h1*av1*Dz)/(ru1/2*cpg*eps1))*Ts(i)+Tg(i-1))/(((h1*av1*Dz)/↙
(ru1/2*cpg*eps1))+1);
    %Mass balance for component
    dx(i)=((x(i-1)-x(i))/Dz)*(u1*Tg(i)/2);
    do(i)=((o(i-1)-o(i))/Dz)*(u1*Tg(i)/2);
    if x(i)<0 %concentration below zero is impossible
        x(i)=0;
    end
    if o(i)<0 %concentration below zero is impossible
        o(i)=0;
    end
    %Heat transfer along solid
```

```
    dTs(i)=(K1/(rs1*cps1*Dz))*((Ts(i+1)-2*Ts(i)+Ts(i-1))/Dz)-((h1*av1)/(rs1*cps1*(1-↙
eps1)))*(Ts(i)-Tg(i));
end
%
%Last section of reactor
i=ns;
%Heat gas balance
Tg(i)=(((h1*av1*Dz)/(ru1/2*cpg*eps1))*Ts(i)+Tg(i-1))/(((h1*av1*Dz)/(ru1/2*cpg*eps1))↙
+1);
%Mass balance for component
dx(i)=((x(i-1)-x(i))/Dz)*(u1*Tg(i)/2);
do(i)=((o(i-1)-o(i))/Dz)*(u1*Tg(i)/2);
if x(i)<0 %concentration below zero is impossible
    x(i)=0;
end
if o(i)<0 %concentration below zero is impossible
    o(i)=0;
end
%Heat transfer along solid
dTs(i)=(K1/(rs1*cps1*Dz))*((-Ts(i)+Ts(i-1))/Dz)-((h1*av1)/(rs1*cps1*(1-eps1)))*(Ts(i)↙
-Tg(i));
%Up date derivate vector
for i=1:ns
    fy(i)=dTs(i);
    fy(i+ns)=dx(i);
    fy(i+2*ns)=do(i);
end
```

```
function fy=m3(t,y)
global ns eps2 K1 K2 rs1 rs2 cps1 cps2 Dz Tg Qre Xm3 Om3
%
%Reactor in absence of the gas flow
fy=zeros(ns,1);
for i=1:ns
    Ts(i)=y(i);      %Solid Temperature
    Tg(i)=Tg(i);     %Gas temperature
    x(i)=Xm3(i);     %VOCs concentration
    o(i)=Om3(i);     %Oxygen concentration
end
%
%INERT
%
%Input setion
%
%Heat transfer along solid
dTs(1)=(K1/(rs1*cps1*Dz))*((Ts(2)-Ts(1))/Dz);
%Gas inside section have same temperature of solid
Tg(1)=Ts(1);
%Concentration does not change
x(1)=x(1);
o(1)=o(1);
if x(1)<0 %concentration below zero is impossible
    x(1)=0;
end
if o(1)<0 %concentration below zero is impossible
    o(1)=0;
end
%
%Along layer of solid inert
for i=2:14
    %Heat transfer along solid
    dTs(i)=(K1/(rs1*cps1*Dz))*((Ts(i+1)-2*Ts(i)+Ts(i-1))/Dz);
    %Gas inside section have same temperature of solid
    Tg(i)=Ts(i);
    %Concentration does not change
    x(i)=x(i);
    o(i)=o(i);
    if x(i)<0 %concentration below zero is impossible
        x(i)=0;
    end
    if o(i)<0 %concentration below zero is impossible
        o(i)=0;
    end

end
%
%Interface inert-catalyst (side inert)
i=15;
%Heat transfer along solid
dTs(i)=(K1/(rs1*cps1*Dz))*((-Ts(i)+Ts(i-1))/Dz)+(K2/(rs1*cps1*Dz))*((-Ts(i)+Ts(i+1))↙
/Dz);
%Gas inside section have same temperature of solid
Tg(i)=Ts(i);
```

```
%Concentration does not change
x(i)=x(i);
o(i)=o(i);
if x(i)<0 %concentration below zero is impossible
    x(i)=0;
end
if o(i)<0 %concentration below zero is impossible
    o(i)=0;
end
%I have assumed that the chemical reaction does not occur
%
%Interface inert-catalyst (side catalyst)
%In dis case
i=16;
%Heat transfer along solid
dTs(i)=(K2/(rs2*cps2*Dz))*((-Ts(i)+Ts(i+1))/Dz)+(K1/(rs2*cps2*Dz))*((-Ts(i)+Ts(i-1))↙
/Dz);
%Gas inside section have same temperature of solid
Tg(i)=Ts(i);
%Concentration does not change
x(i)=x(i);
o(i)=o(i);
if x(i)<0 %concentration below zero is impossible
    x(i)=0;
end
if o(i)<0 %concentration below zero is impossible
    o(i)=0;
end
%
%Along layer of catalyst
%
for i=17:29
    %Heat transfer along solid
    dTs(i)=(K2/(rs2*cps2*Dz))*((Ts(i+1)-2*Ts(i)+Ts(i-1))/Dz);
    %Gas inside section have same temperature of solid
    Tg(i)=Ts(i);
    %Concentration does not change
    x(i)=x(i);
    o(i)=o(i);
    if x(i)<0 %concentration below zero is impossible
        x(i)=0;
    end
    if o(i)<0 %concentration below zero is impossible
        o(i)=0;
    end

end
%
%Interface catalyst-heater (side catalyst)
i=30;
%Heat transfer along solid
dTs(i)=(K2/(rs2*cps2*Dz))*((-Ts(i)+Ts(i-1))/Dz)+((Qre/2)/(rs2*cps2*Dz*(1-eps2)));
%Gas inside section have same temperature of solid
Tg(i)=Ts(i);
%Concentration does not change
```

```
x(i)=x(i);
o(i)=o(i);
if x(i)<0 %concentration below zero is impossible
    x(i)=0;
end
if o(i)<0 %concentration below zero is impossible
    o(i)=0;
end
%
%Central sector (Heater)
i=31;
%Gas temperature is mean value of gas temperature in two near section
Tg(i)=(Tg(i-1)+Tg(i+1))/2;
%Concentration does not change
x(i)=x(i);
o(i)=o(i);
if x(i)<0 %concentration below zero is impossible
    x(i)=0;
end
if o(i)<0 %concentration below zero is impossible
    o(i)=0;
end
%In this section is not present solid
%
%Interface heater-catalyst (side catalyst)
i=32;
%Heat transfer along solid
dTs(i)=(K2/(rs2*cps2*Dz))*((-Ts(i)+Ts(i+1))/Dz)+((Qre/2)/(rs2*cps2*Dz*(1-eps2)));
%Gas inside section have same temperature of solid
Tg(i)=Ts(i);
%Concentration does not change
x(i)=x(i);
o(i)=o(i);
if x(i)<0 %concentration below zero is impossible
    x(i)=0;
end
if o(i)<0 %concentration below zero is impossible
    o(i)=0;
end
%
%Along layer of catalyst
%
for i=33:45
    %Heat transfer along solid
    dTs(i)=(K2/(rs2*cps2*Dz))*((Ts(i+1)-2*Ts(i)+Ts(i-1))/Dz);
    %Gas inside section have same temperature of solid
    Tg(i)=Ts(i);
    %Concentration does not change
    x(i)=x(i);
    o(i)=o(i);
    if x(i)<0 %concentration below zero is impossible
        x(i)=0;
    end
    if o(i)<0 %concentration below zero is impossible
        o(i)=0;
```

```
    end

end
%
%Interface catalyst-inert (side catalyst)
i=46;
%Heat transfer along solid
dTs(i)=(K2/(rs2*cps2*Dz))*((-Ts(i)+Ts(i-1))/Dz)+(K1/(rs2*cps2*Dz))*((-Ts(i)+Ts(i+1))↙
/Dz);
%Gas inside section have same temperature of solid
Tg(i)=Ts(i);
%Concentration does not change
x(i)=x(i);
o(i)=o(i);
if x(i)<0 %concentration below zero is impossible
    x(i)=0;
end
if o(i)<0 %concentration below zero is impossible
    o(i)=0;
end
%
%Interface catalyst-inert (side inert)
i=47;
%Heat transfer along solid
dTs(i)=(K2/(rs1*cps1*Dz))*((-Ts(i)+Ts(i-1))/Dz)+(K1/(rs1*cps1*Dz))*((Ts(i-1)-Ts(i))↙
/Dz);
%Gas inside section have same temperature of solid
Tg(i)=Ts(i);
%Concentration does not change
x(i)=x(i);
o(i)=o(i);
if x(i)<0 %concentration below zero is impossible
    x(i)=0;
end
if o(i)<0 %concentration below zero is impossible
    o(i)=0;
end
%
%Along layer of solid inert
for i=48:60
    %Heat transfer along solid
    dTs(i)=(K1/(rs1*cps1*Dz))*((Ts(i+1)-2*Ts(i)+Ts(i-1))/Dz);
    %Gas inside section have same temperature of solid
    Tg(i)=Ts(i);
    %Concentration does not change
    x(i)=x(i);
    o(i)=o(i);
    if x(i)<0 %concentration below zero is impossible
        x(i)=0;
    end
    if o(i)<0 %concentration below zero is impossible
        o(i)=0;
    end
 end
%
```

```
%Last section of reactor
i=ns;
%Heat transfer along solid
dTs(i)=(K1/(rs1*cps1*Dz))*((-Ts(i)+Ts(i-1))/Dz);
%Gas inside section have same temperature of solid
Tg(i)=Ts(i);
%Concentration does not change
x(i)=x(i);
o(i)=o(i);
if x(i)<0 %concentration below zero is impossible
    x(i)=0;
end
if o(i)<0 %concentration below zero is impossible
    o(i)=0;
end
%Up date derivate vector
for i=1:ns
    fy(i)=dTs(i);
    Xm3(i)=x(i);
    Om3(i)=o(i);
end
```

```
global IN k time1 t Tsw1 Xout TG1 Oout Fout QRE Tmin Tmax Tmean T sint
global React1 React2 VSOF VFILT OUT WSOF TSOF FO
%
%Plant parameter
f=figure(1);
%Graphical name and position
set(f,'name','Parametri','numbertitle','off')
set(f,'units','normalized','position',[0 0.27 0.5 0.73])
%
%Simulation time [%]
if OUT==0
    optf1a=('g');  %If greed simulation has come to the end of time
else
    if OUT==1
        optf1a=('r'); %If red simulated is stopped because system is emergency and↙
reactor cold
    else
        optf1a=('y');  %If yellow simulated is stopped because reactor cold
    end
end
subplot(4,5,1); barh(time1/t*100,optf1a)
title('Time','color',optf1a)
xlim([0 100])
xlabel('%')
%
%Input gas temperature [°C]
subplot(4,5,6); plot(IN(1:k-1,4)-273)
title('Temperature gas input')
ylabel('°C')
xlim([0 length(IN(1:k-1))+10])
xlabel('Time [s]')
%
%Input gas VOCs concentration [%]
subplot(4,5,11); plot(IN(1:k-1,2).*100)
title('Input concentration VOC')
ylabel('%')
xlim([0 length(IN(1:k-1))+10])
xlabel('Time [s]')
%
%Input gas flow rate [Nm3/h
subplot(4,5,16); plot(IN(1:k-1,3))
title('Flow input gas')
ylabel('Nm3/h')
xlim([0 length(IN(1:k-1))+10])
xlabel('Time [s]')
%
%Gas flow rate after blower [Nm3/h
subplot(4,5,2); plot(VSOF(2:end))
title('Flow after blower')
ylabel('Nm3/h')
xlim([0 length(VSOF(2:end))+10])
xlabel('Time [s]')
%
%Blower power [kW]
subplot(4,5, 7); plot(WSOF(2:end)./1000)
```

```
title('Blower work')
ylabel('kW')
xlim([0 length(WSOF(2:end))+10])
xlabel('Time [s]')
%
%Gas temperature after blower [°C]
subplot(4,5, 12); plot(TSOF(2:end)-273)
title('Temperature after blower')
ylabel('°C')
xlim([0 length(TSOF(2:end))+10])
xlabel('Time [s]')
%
%Flow rate through filter [Nm3/h]
subplot(4,5,17); plot(VFILT(2:end))
title('Flow after filter')
ylabel('Nm3/h')
xlim([0 length(VFILT(2:end))+10])
xlabel('Time [s]')
%
%Oxygen flow rate [Nm3/h]
subplot(4,5, 3); plot(FO(2:end))
title('Oxygen flow')
ylabel('Nm3/h')
xlim([0 length(FO(2:end))+10])
xlabel('Time [s]')
%
%Oxygen concentration in gas after it input [%]
subplot(4,5, 8); plot(IN(1:k-1,5).*100)
title('Oxygen conctration')
ylabel('%')
xlim([0 length(IN(1:k-1))+10])
xlabel('Time [s]')
%
%Time between two inversion of flow inside reactor
subplot(4,5, 13); bar(Tsw1)
title('Inversion Time')
ylabel('s')
xlim([0 length(Tsw1)+1])
xlabel('Inversion')
%
%Heat provide by heater
subplot(4,5, 18); plot(QRE(2:end)./1000)
title('Heat of heater')
ylabel('kW')
xlim([0 length(QRE)+1])
xlabel('Time [s]')
%
%Solid temperature inside reactor [°C] (Tmax = maximum temperature; Tmean = mean
%temperature; Tmin = minimum temperature)
subplot(4,5,4); plot(T(2:end), Tmin-273, T(2:end), Tmean-273, T(2:end), Tmax-273)
legend('Tmin','Tmed','Tmax','Location', [0.75 0.95 0.05 0.05])
title('Solid temperatura')
ylabel('°C')
xlim([0 T(end)+1])
xlabel('Time [s]')
```

```
%
%Catalyst state (0 = work correctly; 1 = catalyst sintered)
x9=0;
for i=1:61
x9(i)=Dz*(i-1);
end
subplot(4,5, 9); bar(x9, sint)
title('Catalist state')
xlim([0 max(x9)+0.1])
xlabel('Length [m]')
%
%how occurs the passage of the gas in the reactor in one phase of operation
% 0 = reactor work correctly
% 1 = reactor is bypassed
% 2 = gas pass in wrong direction
% 3 = gas can not pass inside reactor
% 4 = plant is in emergency
subplot(4,5, 14); bar(React1(2:end))
title('Flow state during phase XV12-->XV14')
xlim([0 length(React1)+1])
xlabel('Inversion')
%
%how occurs the passage of the gas in the reactor in other phase of operation
% 0 = reactor work correctly
% 1 = reactor is bypassed
% 2 = gas pass in wrong direction
% 3 = gas can not pass inside reactor
% 4 = plant is in emergency
subplot(4,5, 19); bar(React2(2:end))
title('Flow state during phase XV15-->XV13')
xlim([0 length(React2)+1])
xlabel('Inversion')
%
%Output gas temperature [°C]
subplot(4,5,5); plot(TG1(2:end)-273)
title('Temperature in output gas')
ylabel('°C')
xlim([0 length(TG1)+10])
xlabel('Time [s]')
%
%Output gas VOCs concentration [%]
subplot(4,5,10); plot(Xout(2:end).*100)
title('VOC concentration in output gas')
ylabel('%')
xlim([0 length(Xout)+10])
xlabel('Time [s]')
%
%Output gas oxygen concentration [%]
subplot(4,5,15); plot(Oout(2:end).*100)
title('O2 concentration in output gas')
ylabel('%')
xlim([0 length(Oout)+10])
xlabel('Time [s]')
%
%Output gas flow rate [Nm3/h]
```

```
subplot(4,5,20); plot(Fout(2:end))
title('Flow of output gas')
ylabel('Nm3/h')
xlim([0 length(Fout)+10])
xlabel('Time [s]')
```

```
global All Funz IN Tmax VSOF
%
%State of alarm
f=figure(2);
%Figure name and position
set(f,'name','Controllo','numbertitle','off')
set(f,'units','normalized','position',[0.5 0.27 0.5 0.73])
%
%Evaluation operating state from alarms
for fu=1:22
    if Funz(fu)==0
        opsf2(fu)=('g'); %Alarm works correctly
    else
        opsf2(fu)=('r'); %Alarm is fault
    end
end
%
%AAH01
subplot(5, 4, 1); bar(All(:,1),opsf2(1))
title('AAH01','color',opsf2(1))
xlim([0 length(All)+10])
xlabel('Time [s]')
%
%TAH03
subplot(5, 4, 5); bar(All(:,4),opsf2(4))
title('TAH03','color',opsf2(4))
xlim([0 length(All)+10])
xlabel('Time [s]')
%
%PDAH03
subplot(5, 4, 9); bar(All(:,5),opsf2(5))
title('PDAH03','color',opsf2(5))
xlim([0 length(All)+10])
xlabel('Time [s]')
%
%PAH22
subplot(5, 4, 13); bar(All(:,6),opsf2(6))
title('PAH22','color',opsf2(6))
xlim([0 length(All)+10])
xlabel('Time [s]')
%
%AICA18
subplot(5, 4, 17); bar(All(:,7),opsf2(7))
title('AICA18','color',opsf2(7))
xlim([0 length(All)+10])
xlabel('Time [s]')
%
%TAH11
subplot(5, 4, 2); bar(All(:,10),opsf2(10))
title('TAH11','color',opsf2(10))
xlim([0 length(All)+10])
%
%TAH21
subplot(5, 4, 6); bar(All(:,11),opsf2(11))
title('TAH21','color',opsf2(11))
```

```
xlim([0 length(All)+10])
xlabel('Time [s]')
%
%TAH10
subplot(5, 4, 10); bar(All(:,12),opsf2(12))
title('TAH10','color',opsf2(12))
xlim([0 length(All)+10])
xlabel('Time [s]')
%
%TSH21
subplot(5, 4, 14); bar(All(:,13),opsf2(13))
title('TSH21','color',opsf2(13))
xlim([0 length(All)+10])
xlabel('Time [s]')
%
%TSH10
subplot(5, 4, 18); bar(All(:,14),opsf2(14))
title('TSH10','color',opsf2(14))
xlim([0 length(All)+10])
xlabel('Time [s]')
%
%TAHH11
subplot(5, 4, 3); bar(All(:,15),opsf2(15))
title('TAHH11','color',opsf2(15))
xlim([0 length(All)+10])
xlabel('Time [s]')
%
%TAHH10
subplot(5, 4, 7); bar(All(:,16),opsf2(16))
title('TAHH10','color',opsf2(16))
xlim([0 length(All)+10])
xlabel('Time [s]')
%
%TSHH11
subplot(5, 4, 11); bar(All(:,17),opsf2(17))
title('TSHH11','color',opsf2(17))
xlim([0 length(All)+10])
xlabel('Time [s]')
%
%TSHH10
subplot(5, 4, 15); bar(All(:,18),opsf2(18))
title('TSHH10','color',opsf2(18))
xlim([0 length(All)+10])
xlabel('Time [s]')
%
%TAL10
subplot(5, 4, 4); bar(All(:,19),opsf2(19))
title('TAL10','color',opsf2(19))
xlim([0 length(All)+10])
xlabel('Time [s]')
%
%TSL10
subplot(5, 4, 8); bar(All(:,20),opsf2(20))
title('TSL10','color',opsf2(20))
xlim([0 length(All)+10])
```

```
xlabel('Time [s]')
%
%TALL10
subplot(5, 4, 12); bar(All(:,21),opsf2(21))
title('TALL10','color',opsf2(21))
xlim([0 length(All)+10])
xlabel('Time [s]')
%
%AIA19
subplot(5, 4, 20); bar(All(:,22),opsf2(22))
title('AIA19','color',opsf2(22))
xlim([0 length(All)+10])
xlabel('Time [s]')
%
```

```
%
% Solid temperature trend in the reactor
%
global ns Tsprof Dz
for i1=1:ns %Reactor section
    l(i1)=i1*Dz;
end
hold on
Tsp1=[];
Tsp1=Tsprof(:,1:30)-273;
l1=[];
l1=l(1:30);
figure(5)
[a b]=size(Tsp1);
Nn=1;
for i2=1:a %Time point present
    Nn(i2)=i2;
end
[X,Y] = meshgrid(Nn(2:end),l1);
X=X';
Y=Y';
surface(X,Y,Tsp1(2:end,:))
shading interp
xlabel('time')
ylabel('z')
zlabel('T')
Tsp2=[];
Tsp2=Tsprof(:,32:61)-273;
l2=[];
l2=l(32:61);
figure(5)
[a b]=size(Tsp2);
Nn=1;
for i3=1:a
    Nn(i3)=i3;
end
[X,Y] = meshgrid(Nn(2:end),l2);
X=X';
Y=Y';
surface(X,Y,Tsp2(2:end,:))
shading interp

xlabel('time [s]', 'FontSize',16)
ylabel('length [m]', 'FontSize',16)
zlabel('Temperature [°C]   ', 'FontSize',16)
xlim([0 5000])
ylim([0 0.7])
zlim([min(min(Tsprof(2:end,:)-273)-1) max(max(Tsprof(2:end,:)-273)+1)])
colorbar
az = 45;
el = 45;
view(az, el);
set(gca, 'FontSize', 16)
str = {'Temperature [°C]   '};
annotation('textbox', [.869 .926, .135, .034],'FontSize', 16, 'LineStyle' , 'none',↙
```

```
...
            'String', str);


hold off
```

```
%
%Evaluate management costs
%
global efilt eox esof eval ereat esint eelet eout tygua efer tfer Psofnorm
global Det sof emer filt ox sint React1 React2 crea Qnorm QRE IN Xout CKvar
global WSOF
%
%
costo=[];
costo1=[];
%
%Cost to restor blower [€]
if sof==0
    costo1(1)=0;
else
    costo1(1)=esof;
end
%
%Energy cost for blower
%
%Energy cost for normal function before time mathematically modeled
WSOF1=WSOF./1000;
Psofnorm=mean(WSOF1(15:tsgua-10));
es1=tygua*Psofnorm;
%
%Energy cost for time mathematically modeled
WSOF1=WSOF./1000;
es2=sum(WSOF1(2:end).*(Det/3600));
%
%After time mathematically modeled
if emer==1
    %If plant have emergency, after restart to work corectly
    es3=(8760-tygua-tfer-(time1/3600))*Psofnorm;
else
    %If plant have not emergency continue to consume energy as in the last
    %part of the simulation
    es4=mean(WSOF1(end-1000:end));
    es3=es4*(8760-tygua-(time1/3600));
end
%Energy cost for blower [€]
estot=es1+es2+es3;
costo1(2)=estot*eelet;
%
%Cost to restor filter [€]
if filt==0
    costo1(3)=0;
else
    costo1(3)=efilt;
end
%
%Cost restor oxygen input [€]
if ox==0
    costo1(4)=0;
else
    costo1(4)=eox;
```

```
end
%
%Reactor
%Cost restor valve [€]
if max(React1(2:end))==0 && sum(React2(2:end))==0
    costo1(5)=0;
else
    if max(React1(2:end))==4 || sum(React2(2:end))==4
        costo1(5)=0;
    else
        costo1(5)=eval;
    end
end
%Cost restor catalyst [€]
if sum(sint)==0
    costo1(6)=0;
else
    costo1(6)=esint;
end
%Cost restor reactor temperature control [€]
if crea==0
    costo1(7)=0;
else
    costo1(7)=ereat;
end
%
%Energy cost for heater
%
%Energy cost for normal function before time mathematically modeled
QRE1=QRE./1000;
Qnorm=mean(QRE1(15:tsgua-10))
en1=tygua*Qnorm;
%
%Energy cost for time mathematically modeled
en2=sum(QRE1(2:end).*(Det/3600));
%
%After time mathematically modeled
if emer==1
    %If plant have emergency, after restart to work correctly
    en3=(8760-tygua-tfer-(time1/3600))*Qnorm;
else
    %If plant have not emergency continue to consume energy as in the last
    %part of the simulation
    en4=mean(QRE1(end-1000:end));
    en3=en4*(8760-tygua-(time1/3600));
end
%Energy cost for heater [€]
erisc=en1+en2+en3;
costo1(8)=erisc*eelet;
%
%Cost for missed VOCs reduction [€]
if emer==1
    costo1(9)=0;
else
    if mean(Xout(end-1000:end))>=(CKvar/100)*mean(IN(end-1000:end,2))
```

```
        costo1(9)=eout;
    else
        costo1(9)=0;
    end
end
%
%Cost for emergency [€]
if emer==1
    costo1(10)=efer;
else
    costo1(10)=0;
end
%
%Evaluation global management cost
costo=sum(costo1);
```

```
%
%Control congruency logical analysis
%
global CK1 CHECK IN2 TSOF VSOF VFILT TING Xout sint Tmax CKvar TIN1 XIN1
global VIN1 oset Tre emer Oout
%Prepare variable used
CK2=[];
CK3=[];
CHECK=[];
% CREA VALORI PER CONTROLLO USO MEDIATO SUGLI ULTI M VALORI
%
M=1000;
CK2(1)=mean(IN2(end-M:end,4)); %Mean gas input temperature
CK2(2)=mean(IN2(end-M:end,2)); %Mean gas input VOCs concentration
CK2(3)=mean(IN2(end-M:end,3)); %Mean gas input flow rate
CK2(4)=mean(TSOF(end-M:end)); %Mean temperature after blower
CK2(5)=mean(VSOF(end-M:end)); %Mean flow after blower
CK2(6)=mean(VFILT(end-M:end)); %Mean gas flow through filter
CK2(7)=mean(Oout(end-M-1:end-1)); %Mean gas output oxygen concentration
CK2(8)=mean(TING(end-M:end)); %Mean temperature of gas in reactor input
CK2(10)=mean(Xout(end-M:end)); %Mean gas output VOCs concentration
CK2(9)=sum(sint); %State of catalyst
CK2(11)=mean(Tmax(end-M:end)); %Mean maximum temperature inside reactor
CKvar=CKvar/100;
%
%Input condition
%Temperature
if emer>0 && (CK1(1)==0)
    CK3(1)=0;
else
    if CK2(1)<(TIN1*(1+CKvar)) && CK2(1)>(TIN1*(1-CKvar))
        CK3(1)=20;
    else
        if CK2(1)>(TIN1*(1+CKvar))
            CK3(1)=21;
        else
            CK3(1)=-21;
        end
    end
end
%VOCs concentration
if emer>0 && (CK1(2)==0)
    CK3(2)=0;
else
    if CK2(2)<(XIN1*(1+CKvar)) && CK2(2)>(XIN1*(1-CKvar))
        CK3(2)=22;
    else
        if CK2(2)>(XIN1*(1+CKvar))
            CK3(2)=23;
        else
            CK3(2)=-23;
        end
    end
end
%Flow rate
```

```
if emer>0 && (CK1(3)==0)
    CK3(3)=0;
else
    if CK2(3)<(VIN1*(1+CKvar)) && CK2(3)>(VIN1*(1-CKvar))
        CK3(3)=24;
    else
        if CK2(3)>(VIN1*(1+CKvar))
            CK3(3)=25;
        else
            CK3(3)=-25;
        end
    end
end
%
%Blower
%Gas temperature after blower
if emer>0 && (CK1(4)==0)
    CK3(4)=0;
else
    if CK2(4)<((TIN1+8)*(1+CKvar)) && CK2(4)>((TIN1+7)*(1-CKvar))
        CK3(4)=80;
    else
        if CK2(4)>((TIN1+8)*(1+CKvar))
            CK3(4)=81;
        else
            CK3(4)=-81;
        end
    end
end
%Gas flow rate after blower
if emer>0 && (CK1(5)==0)
    CK3(5)=0;
else
    if CK2(5)<(VIN1*(1+CKvar)) && CK2(5)>(VIN1*(1-CKvar))
        CK3(5)=84;
    else
        if CK2(5)>(VIN1*(1+CKvar))
            CK3(5)=85;
        else
            CK3(5)=-85;
        end
    end
end
%
%Filter
%Gas flow rate after filter
if emer>0 && (CK1(6)==0)
    CK3(6)=0;
else
    if CK2(6)<(VIN1*(1+CKvar)) && CK2(6)>(VIN1*(1-CKvar))
        CK3(6)=119;
    else
        if CK2(6)>(VIN1*(1+CKvar))
            CK3(6)=120;
        else
```

```
            CK3(6)=-120;
        end
    end
end
%
%Oxygen input
if emer>0 && (CK1(7)==0)
    CK3(7)=0;
else
    if CK2(7)<oset*(1+CKvar) && CK2(7)>oset*(1-CKvar)
        CK3(7)=179;
    else

        if CK2(7)>oset*(1+CKvar)
            CK3(7)=180;
        else
            CK3(7)=-180;
        end
        if react1==3 || react2==3
            CK3(7)=179;
        end
    end
end
%
%Reactor
%Reactor temperature
if emer>0 && (CK1(8)==0)
    CK3(8)=0;
else
    if CK2(8)<((TIN1+8)*(1+CKvar)) && CK2(8)>((TIN1+7)*(1-CKvar))
        CK3(8)=210;
    else
        if CK2(8)>((TIN1+8)*(1+CKvar))
            CK3(8)=211;
        else
            CK3(8)=-211;
        end
    end
end
%Output VOCs concentration
if CK2(10)>(XIN1*CKvar)
    CK3(10)=-650;
else
   CK3(10)=650;
end
%
%Reactor condition
if emer>0 %Emergency
    CK3(9)=-4698;
    if (CK1(9)==4698 || CK1(9)==-602) && Funz (22)==0
        CK3(9)=CK1(9);
    end
else
    if CK2(9)>=1 %Catalyst sintered
        CK3(9)=4698;
```

```
    else
        if CK2(11)<=Tre %Reactor shout down
            CK3(9)=-602;
        end
    end
end
%
%Comparison of the results obtained from the phenomenological modeling with
%the indications of logical modeling
for i=1:10
    if CK1(i)==CK3(i)
        CHECK(i)=0;  %Value is coherent in logical model
    else  %Logical model at this point is not coherent with the physics of the↙
process
        if CK1(i)==0
            CHECK(i)=abs(CK3(i));
        else
            CHECK(i)=abs(CK1(i));
        end
    end
end
```