

Combination of reactingFoam and chtMultiRegionFoam as a first step toward creating a multiRegionReactingFoam, suitable for solid/gas phase reactions

Seyed Morteza Mousavi

Department of Energy Sciences, Division of Fluid Dynamics,
Lund University,
Lund, Sweden

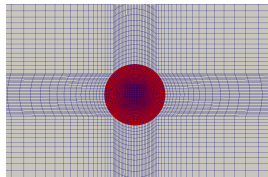
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Contents:

- Introduction
- Theory
- Tutorials
- Implementation
- Using the new solver

Background, solid fuel combustion

- Combustion mainly happens in gas phase
- Solid fuel is converted to gas first
- Intraparticle gradients depend on size
 - Small particles ($Bi \ll 1$)
 - **Large particles** ($Bi > 1$)



Motivation for multiRegionReactingFoam

- First step to model the flow and reactions inside a reacting porous particle
- reactingFoam is available for fluid region
- chtMultiRegionFoam is available, which couples multiple regions
- Several tasks to obtain a model for solid fuel combustion:
 - **Add a solid region to the reactingFoam solver**
 - **Solve energy equation for solid**
 - **Appropriate BC to couple E-equations**
 - Solve pyrolysis and Darcy equations inside porous media
 - Appropriate BC to couple U , p , Y_i equations

Fluid region governing equations

continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho U) = 0 \quad (1)$$

momentum equation

$$\frac{\partial}{\partial t}(\rho U) + \nabla \cdot (\rho U U) = -\nabla p + \nabla \cdot \tau \quad (2)$$

species transport equation

$$\frac{\partial}{\partial t}(\rho Y_i) + \nabla \cdot (\rho U Y_i) = \nabla \mu_{eff} \nabla Y_i + \dot{R}_i \quad (3)$$

and energy equation

$$\frac{\partial}{\partial t}(\rho h) + \nabla \cdot (\rho U h) + \frac{\partial}{\partial t}(\rho K) + \nabla \cdot (\rho U K) - \frac{\partial p}{\partial t} = \nabla \alpha_{eff} \nabla h + \dot{R}_{heat} \quad (4)$$

Solid region governing equations

Solid energy equation (heat conduction)

$$\frac{\partial}{\partial t}(\rho h) = \nabla \alpha_{eff} \nabla h \quad (5)$$

DLR_A_LTS tutorial case

```

0
├── alphabet
├── CH4
├── epsilon
├── G
├── H2
├── H2O
├── k
├── N2
├── nut
├── O2
├── p
├── T.orig
├── U
├── Ydefault
├── Allclean
├── Allrun
├── chenkin
├── │
├── │ grimech30.dat
├── │ thermo30.dat
├── │ transportProperties
├── constant
├── │ chemistryProperties
├── │ chemistryProperties.test
├── │ combustionProperties
├── │ g
├── │ reactionsCRI
├── │ thermo.compressibleGasCRI
├── │ thermophysicalProperties
├── │ turbulenceProperties
├── system
├── │ blockMeshDict
├── │ controlDict
├── │ decomposeParDict
├── │ fvSchemes
├── │ fvSolution
├── │ setFieldsDict

```

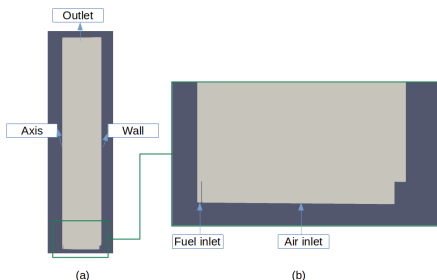


Figure: Geometry of the DLR_A_LTS case.

Figure: The contents of the DLR_A_LTS tutorial case.

Initialize and run the case

Get the case:

```
run
cp -r $FOAM_TUTORIALS/combustion/reactingFoam/RAS/DLR_A_LTS/ .
cd DLR_A_LTS
```

Get a global reaction mechanism:

```
mkdir constant/BACKUP

mv constant/{chemistryProperties,thermophysicalProperties,\
reactionsGRI,thermo.compressibleGasGRI} constant/BACKUP

cp $FOAM_TUTORIALS/combustion/reactingFoam/RAS/membrane/constant/{chemistryProperties,\
thermophysicalProperties,reactions,thermo.compressibleGas} constant/

sed -i s/"chemistry .*/"chemistry on;"/g constant/chemistryProperties
```

Run the case:

```
./Allrun
```

Some results

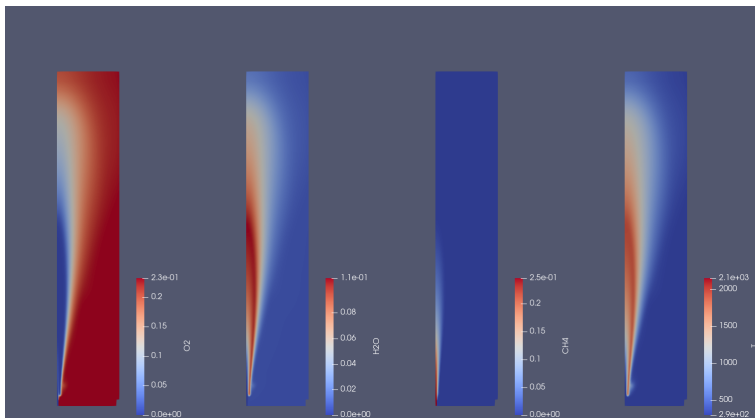


Figure: Final results of the DLR_A_LTS case using a simple global reaction mechanism. From left to right, O_2 mass fraction, H_2O mass fraction, CH_4 mass fraction, and temperature distribution.

multiRegionHeater tutorial case

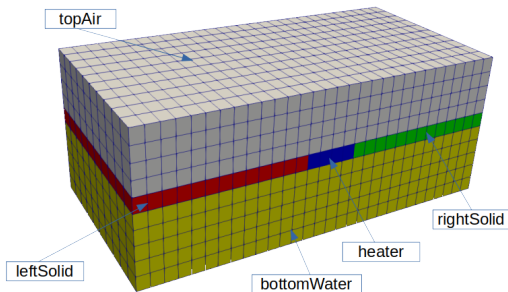
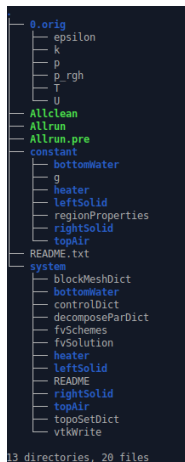


Figure: Geometry of the multiRegionHeater case.

Figure: Contents.

multiRegionHeater tutorial case

0/heater/T

```
heater_to_leftSolid
{
    type compressible::turbulent\
        TemperatureCoupledBaffleMixed;
    value          uniform 300;
    Tnbr           T;
    kappaMethod     solidThermo;
    thicknessLayers ( 0.001 );
    kappaLayers     ( 0.0005 );
}
```

constant/regionProperties

```
regions
(
    fluid (bottomWater topAir)
    solid (heater leftSolid rightSolid)
);
```

system/topoSetDict

```
actions
(
    ...
    // leftSolid
    {
        name      leftSolidCellSet;
        type      cellSet;
        action     new;
        source     boxToCell;
        box        (-100 0 -100) (-0.01001 0.00999 100);
    }
    {
        name      leftSolid;
        type      cellZoneSet;
        action     new;
        source     setToCellZone;
        set        leftSolidCellSet;
    }
    ...
)
```

Initialize and run the case

Get the case and run:

```
run
cp -r $FOAM_TUTORIALS/heatTransfer/chtMultiRegionFoam/multiRegionHeater/ .
cd multiRegionHeater
./Allrun
```

Allrun script :

```
runApplication ./Allrun.pre
# Decompose
runApplication decomposePar -allRegions
# Run
runParallel $(getApplication)
# Reconstruct
runApplication reconstructPar -allRegions
```

Allrun.pre script :

```
runApplication blockMesh
runApplication topoSet

# Restore initial fields
restore0Dir

runApplication splitMeshRegions -cellZones -overwrite
# Remove fluid fields from solid regions
# (important for post-processing)
...
```

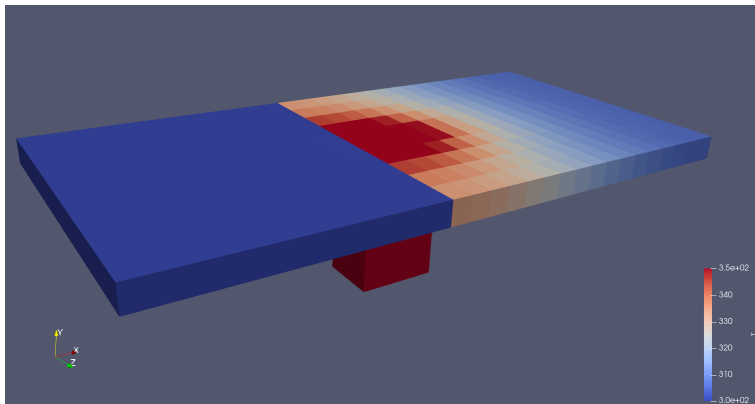


Figure: The final temperature of the solid regions in the multiRegionHeater tutorial case.

Look into reactingFoam.C

Go to case directory

```
sol  
cd combustion/reactingFoam
```

Included libraries

```
#include "fvCFD.H"  
#include "turbulentFluidThermoModel.H"  
#include "psiReactionThermo.H"  
#include "CombustionModel.H"  
#include "multivariateScheme.H"  
#include "pimpleControl.H"  
#include "pressureControl.H"  
#include "fvOptions.H"  
#include "localEulerDdtScheme.H"  
#include "fvcSmooth.H"
```

Look into reactingFoam.C

To use LTS in a case, we need

```
ddtSchemes
{
    default          localEuler;
}
```

Back to the reactingFoam.C

```
int main(int argc, char *argv[])
{
    argList::addNote
    (
        "Solver for combustion with chemical reactions"
    );

    #include "postProcess.H"

    #include "addCheckCaseOptions.H"
    #include "setRootCaseLists.H"
```


Look into reactingFoam.C

```
#include "createTime.H"           // runTime
#include "createMesh.H"           // mesh
#include "createControl.H"        // pimple
#include "createTimeControls.H"   // adjustTimeStep, maxCo, maxDeltaT
#include "initContinuityErrs.H"   // cumulativeContErr
#include "createFields.H"
#include "createFieldRefs.H"
```

Look into createFields.H

```
#include "createRDeltaT.H" \\ bool LTS = fv::localEulerDdt::enabled(mesh);

Info<< "Reading thermophysical properties\n" << endl;
autoPtr<psiReactionThermo> pThermo(psiReactionThermo::New(mesh));
psiReactionThermo& thermo = pThermo();
thermo.validate(args.executable(), "h", "e");

basicSpecieMixture& composition = thermo.composition();
PtrList<volScalarField>& Y = composition.Y();

const word inertSpecie(thermo.get<word>("inertSpecie"));
if (!composition.species().found(inertSpecie))
{
    FatalIOErrorIn(args.executable().c_str(), thermo)
        << "Inert specie " << inertSpecie << " not found in available species "
        << composition.species() << exit(FatalIOError);
}
```

Look into createFields.H

The ρ , p , U , and ϕ variables are created similar to other solvers. Then:

```
autoPtr<compressible::turbulenceModel> turbulence
(
    compressible::turbulenceModel::New
    (
        rho,
        U,
        phi,
        thermo
    )
);
autoPtr<CombustionModel<psiReactionThermo>> reaction
(
    CombustionModel<psiReactionThermo>::New(thermo, turbulence())
);
```

Look into createFields.H

```
volScalarField Qdot
(
    IOobject
    (
        "Qdot",
        runTime.timeName(),
        mesh,
        IOobject::READ_IF_PRESENT,
        IOobject::AUTO_WRITE
    ),
    mesh,
    dimensionedScalar(dimEnergy/dimVolume/dimTime, Zero)
);

#include "createDpdt.H"
#include "createK.H"
#include "createMRF.H"
#include "createFvOptions.H"
```

Look into createFieldRefs.H

```
const volScalarField& psi = thermo.psi();
const volScalarField& T = thermo.T();
const label inertIndex(composition.species()[inertSpecie]);
```

(Why these references are separated from others?)

Back to the main file:

```
turbulence->validate();

if (!LTS)
{
    #include "compressibleCourantNo.H"
    #include "setInitialDeltaT.H"
}
```

Look into reactingFoam.C

```
Info<< "\nStarting time loop\n" << endl;

while (runTime.run())
{
    #include "readTimeControls.H"

    if (LTS)
    {
        #include "setRDeltaT.H"
    }
    else
    {
        #include "compressibleCourantNo.H"
        #include "setDeltaT.H"
    }

    ++runTime;

    Info<< "Time = " << runTime.timeName() << nl << endl;
```

Look into reactingFoam.C

```
#include "rhoEqn.H"
while (pimple.loop())
{
    #include "UEqn.H"
    #include "YEqn.H"
    #include "EEqn.H"
    // --- Pressure corrector loop
    while (pimple.correct())
    {
        if (pimple.consistent())
        {
            #include "pcEqn.H"
        }
        else
        {
            #include "pEqn.H"
        }
    }
    if (pimple.turbCorr())
    {
        turbulence->correct();
    }
}
rho = thermo.rho();
runTime.write();
runTime.printExecutionTime(Info);
```

Look into equations I

rhoEqn.H

```
fvScalarMatrix rhoEqn
(
    fvm::ddt(rho)
    + fvc::div(phi)
    ==
    fvOptions(rho)
);
```

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho U) = 0$$

UEqn.H

```
tmp<fvVectorMatrix> tUEqn
(
    fvm::ddt(rho, U) + fvm::div(phi, U)
    + MRF.DDt(rho, U)
    + turbulence->divDevRhoReff(U)
    ==
    fvOptions(rho, U)
);
...
if (pimple.momentumPredictor())
    solve(UEqn == -fvc::grad(p));
```

$$\frac{\partial}{\partial t}(\rho U) + \nabla \cdot (\rho U U) = -\nabla p + \nabla \cdot \tau$$

$$\tau = \mu \left[(\nabla U + \nabla U^T) - \frac{2}{3} \nabla \cdot U I \right]$$

Look into equations II

YEqn.H

```
fvScalarMatrix YiEqn
(
    fvm::ddt(rho, Yi)
    + mvConvection->fvmDiv(phi, Yi)
    - fvm::laplacian(turbulence->muEff(), Yi)
    ==
    reaction->R(Yi)
    + fvOptions(rho, Yi)
);
```

$$\frac{\partial}{\partial t}(\rho Y_i) + \nabla \cdot (\rho U Y_i) = \nabla \mu_{eff} \nabla Y_i + \dot{R}_i$$

Look into equations III

EEqn.H

```
fvScalarMatrix EEqn
(
    fvm::ddt(rho, he) + mvConvection->fvmDiv(phi, he)
    + fvc::ddt(rho, K) + fvc::div(phi, K)
    + (
        he.name() == "e"
        ? fvc::div
        (
            fvc::absolute(phi/fvc::interpolate(rho), U),
            p,
            "div(phiv,p)"
        )
        : -dpdt
    )
    - fvm::laplacian(turbulence->alphaEff(), he)
    ==
    Qdot
    + fvOptions(rho, he)
);
```

$$\frac{\partial}{\partial t}(\rho h) + \nabla(\rho U h) + \frac{\partial}{\partial t}(\rho K) + \nabla(\rho U K) - \frac{\partial p}{\partial t} = \nabla \alpha_{eff} \nabla h + \dot{R}_{heat}$$

Look into chtMultiRegionFoam.C

Go to the directory of the solver

```
sol
cd heatTransfer/chtMultiRegionFoam/
```

Among libraries:

```
#include "solidRegionDiffNo.H"
#include "regionProperties.H"
```

Inside regionProperties class:

```
// Member Functions
//- Total count of all region names.
label count() const;
//- The region names. Sorted by region type.
wordList names() const;
//- The region names in sorted order.
wordList sortedNames() const;
```

Inside the case directory:
constant/regionProperties
file

```
regions
(
    fluid (bottomWater topAir)
    solid (heater leftSolid rightSolid)
);
```

Look into chtMultiRegionFoam.C

Parts of code included in the main function:

```
int main(int argc, char *argv[])
{
    ...
    #define NO_CONTROL
    #define CREATE_MESH createMeshesPostProcess.H
    #include "postProcess.H"
    ...
    #include "createMeshes.H"                // fluidRegions and solidRegions
    ...
    #include "readSolidTimeControls.H"       // maxDi
    #include "compressibleMultiRegionCourantNo.H" // coNum
    #include "solidRegionDiffusionNo.H"     // DiNum
    #include "setInitialMultiRegionDeltaT.H" // call to runTime.setDeltaT
}
```

Inside createMeshes.H

```
regionProperties rp(runTime);

#include "createFluidMeshes.H"
#include "createSolidMeshes.H"
```

Look into chtMultiRegionFoam.C

Right after setInitialMultiRegionDeltaTT, is the main loop:

```
while (runTime.run())
{
    #include "readTimeControls.H"
    #include "readSolidTimeControls.H"
    #include "readPIMPLEControls.H"

    #include "compressibleMultiRegionCourantNo.H"
    #include "solidRegionDiffusionNo.H"
    #include "setMultiRegionDeltaT.H"
    ...
}
```

How to couple EEqn in two regions?

Find the code for turbulentTemperatureCoupledBaffleMixed:

```
src
find . -iname "turbulentTemperatureCoupledBaffleMixed"
```

Inside turbulentTemperatureCoupledBaffleMixedFvPatchScalarField.H:

Description

Mixed boundary condition for temperature, to be used for heat-transfer on back-to-back baffles. Optional thin thermal layer resistances can be specified through thicknessLayers and kappaLayers entries.

...

Example of the boundary condition specification:

```
<patchName>
{
    type                compressible::turbulentTemperatureCoupledBaffleMixed;
    Tnbr                T;
    thicknessLayers      (0.1 0.2 0.3 0.4);
    kappaLayers          (1 2 3 4);
    kappaMethod          lookup;
    kappa                kappa;
    value                uniform 300;
}
```

Look into turbulentTemperatureCoupledBaffleMixedFvPatchScalarField.H

```
class turbulentTemperatureCoupledBaffleMixedFvPatchScalarField
:
    public mixedFvPatchScalarField,
    public temperatureCoupledBase
{
    // Private data
    //- Name of field on the neighbour region
    const word TnbrName_;
    //- Thickness of layers
    scalarList thicknessLayers_;
    //- Conductivity of layers
    scalarList kappaLayers_;
    //- Total contact resistance
    scalar contactRes_;

public:
    //- Runtime type information
    TypeName("compressible::turbulentTemperatureCoupledBaffleMixed");
    // Constructors
    ...
    // Member functions
    //- Update the coefficients associated with the patch field
    virtual void updateCoeffs();
    //- Write
    virtual void write(Ostream&) const;
}
```

How mixed boundaries work in OF? (mixedFvPatchField.H)

$$x_p = wx + (1 - w) \left(x_c + \frac{\nabla_{\perp} x}{\Delta} \right)$$

where

variable	Access name to modify	Description
x_p	-	patch values
x_c	-	patch internal cell values
x	refValue	reference value
$\nabla_{\perp} x$	refGrad	reference gradient
w	valueFraction	weight field
Δ	-	inverse distance from face centre to internal cell centre

For instance:

$w = 1$: fixedValue BC

$w = 0$: fixedGradient BC

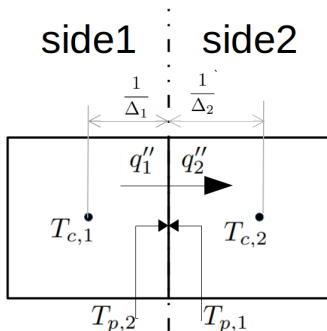
Inside updateCoeffs()

```

this->refValue() = nbrIntFld();
this->refGrad() = 0.0;
this->valueFraction() = nbrKDelta()/(nbrKDelta() + myKDelta());

mixedFvPatchScalarField::updateCoeffs();

```



$$x = refValue = T_{c,2}$$

$$\nabla_{\perp} x = refGrad = 0.0$$

$$w = valueFraction = \frac{k_2 \Delta_2}{k_1 \Delta_1 + k_2 \Delta_2}$$

Calculating the patch values

$$x_p = wx + (1 - w) \left(x_c + \frac{\nabla_{\perp} x}{\Delta} \right)$$

$$x = refValue = T_{c,2}$$

$$\nabla_{\perp} x = refGrad = 0.0$$

$$w = valueFraction = \frac{k_2 \Delta_2}{k_1 \Delta_1 + k_2 \Delta_2}$$

Therefore we have:

$$T_p = \frac{k_2 \Delta_2}{k_1 \Delta_1 + k_2 \Delta_2} T_{c,2} + \left(\frac{k_1 \Delta_1}{k_1 \Delta_1 + k_2 \Delta_2} \right) (T_{c,1} + 0.0)$$

$$\rightarrow T_p = \frac{k_1 \Delta_1 T_{c,1} + k_2 \Delta_2 T_{c,2}}{k_1 \Delta_1 + k_2 \Delta_2}$$

Implementing multiRegionReactingFoam

Start from a fresh copy of reactingFoam.

```
foam
cp --parents -r applications/solvers/combustion/reactingFoam/ $WM_PROJECT_USER_DIR
cd $WM_PROJECT_USER_DIR/applications/solvers/combustion/reactingFoam/
rm -r rhoReacting*
```

Change filenames and make sure you can compile.

```
cd ..
mv reactingFoam multiRegionReactingFoam
cd multiRegionReactingFoam
mv reactingFoam.C multiRegionReactingFoam.C
sed -i s/FOAM_APPBIN/FOAM_USER_APPBIN/g Make/files
sed -i s/reactingFoam/multiRegionReactingFoam/g Make/files
wclean
wmake
```

Implementing multiRegionReactingFoam

Add following libraries to multiRegionReactingFoam.C

```
// Solid region libraries
#include "solidRegionDiffNo.H"
#include "solidThermo.H"
```

In the main function, modify the .H files.

```
// To be able to use postProcess
#define CREATE_MESH createMeshes.H
#include "postProcess.H"

#include "addCheckCaseOptions.H"
#include "setRootCaseLists.H"
#include "createTime.H"
// To create more than one mesh
#include "createMeshes.H"
#include "createControl.H"
#include "createTimeControls.H"
// To read the max diffusion number
#include "readSolidTimeControls.H"
#include "initContinuityErrs.H"
#include "createFields.H"
#include "createFieldRefs.H"
```

Implementing multiRegionReactingFoam

Create a new file named createMeshes.H.

```
Foam::Info
<< "Create fluid mesh for time = "
<< runTime.timeName() << Foam::nl << Foam::endl;
Foam::fvMesh mesh
(
    Foam::IOobject
    (
        "fluid",
        runTime.timeName(),
        runTime,
        Foam::IOobject::MUST_READ
    )
);
Foam::Info
<< "Create pyrolysis mesh for time = "
<< runTime.timeName() << Foam::nl << Foam::endl;
Foam::fvMesh pyrolysisMesh
(
    Foam::IOobject
    (
        "pyrolysisRegion",
        runTime.timeName(),
        runTime,
        Foam::IOobject::MUST_READ
    )
);
```

Implementing multiRegionReactingFoam

Copy some files from chtMultiRegionFoam solver to solid sub-directory.

```
mkdir solid
cp $FOAM_SOLVERS/heatTransfer/chtMultiRegionFoam/solid/readSolidTimeControls.H solid/
cp $FOAM_SOLVERS/heatTransfer/chtMultiRegionFoam/solid/solidRegionDiffNo.H solid/
cp $FOAM_SOLVERS/heatTransfer/chtMultiRegionFoam/solid/solidRegionDiffNo.C solid/
cp $FOAM_SOLVERS/heatTransfer/chtMultiRegionFoam/solid/solidRegionDiffusionNo.H solid/
cp $FOAM_SOLVERS/heatTransfer/chtMultiRegionFoam/include/setMultiRegionDeltaT.H solid/
```

Back to main function in main file, replace the if (LTS) block with the following:

```
if (LTS)
{
    #include "setRDeltaT.H"
}
else
{
    #include "compressibleCourantNo.H"
    // To include solidRegion in decision over deltaT
    #include "solidRegionDiffusionNo.H"
    #include "setMultiRegionDeltaT.H"
}
```

Implementing multiRegionReactingFoam

Add the following lines to main loop, after EEqn.H.

```
// To solve the solid energy equation
#include "solidEEqn.H"
```

Create a new file named solidEEqn.H in the solid sub-directory containing the following code.

```
{
    volScalarField& h = pyroThermo.he();
    pyroRho = pyroThermo.rho();
    fvScalarMatrix hEqn
    (
        fvm::ddt(pyroRho, h)
        - fvm::laplacian(pyroThermo.alpha(), h)
        ==
        fvOptions(pyroRho, h)
    );
    hEqn.relax();
    fvOptions.constrain(hEqn);
    hEqn.solve();
    fvOptions.correct(h);
    pyroThermo.correct();
    Info<< "Solid Min/max T:" << min(pyroThermo.T()).value() << " "
        << max(pyroThermo.T()).value() << endl;
}
```

Implementing multiRegionReactingFoam

Create another empty file named createSolidFields.H in the solid sub-directory and add following.

```
Info<< "Reading solid thermophysical properties\n" << endl;
autoPtr<solidThermo> pPyroThermo(solidThermo::New(pyrolysisMesh));
solidThermo& pyroThermo = pPyroThermo();
```

```
volScalarField pyroRho
(
    IOobject
    (
        "solidRho",
        runTime.timeName(),
        pyrolysisMesh
    ),
    pyroThermo.rho()
);
```

Add the following two lines to the last line of the original createFields.H

```
// To create the solid fields
#include "createSolidFields.H"
```


Implementing multiRegionReactingFoam

Replace the contents of the solid/solidRegionDiffusionNo.H file with the following.

```
scalar DiNum = -GREAT;

{
    tmp<volScalarField> magKappa;
    magKappa = pyroThermo.kappa();

    tmp<volScalarField> tcp = pyroThermo.Cp();
    const volScalarField& cp = tcp();

    tmp<volScalarField> trho = pyroThermo.rho();
    const volScalarField& rho = trho();

    DiNum = solidRegionDiffNo
    (
        pyrolysisMesh,
        runTime,
        rho*cp,
        magKappa()
    );
}
```

Implementing multiRegionReactingFoam

Modify Make/files

```
solid/solidRegionDiffNo.C
multiRegionReactingFoam.C
```

```
EXE = $(FOAM_USER_APPBIN)/multiRegionReactingFoam
```

Add these to the Make/options

```
EXE_INC = \
    -I./solid \
    -I$(LIB_SRC)/thermophysicalModels/solidThermo/lnInclude \
    ...
```

```
EXE_LIBS = \
    -lsolidThermo \
    ...
```

Thats it, the code should be ready now! Try compiling it.

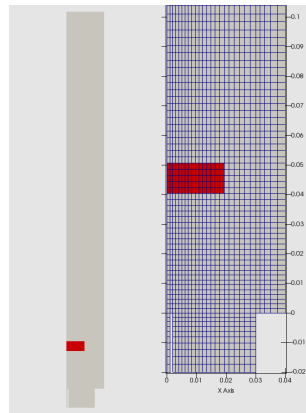
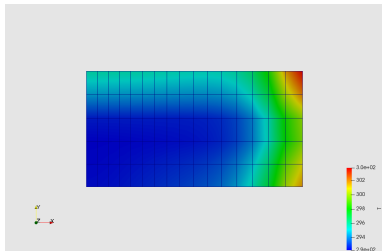
```
wclean
wmake
```

Simple tutorial for multiRegionReactingFoam

Simply go to the case directory and
run it:

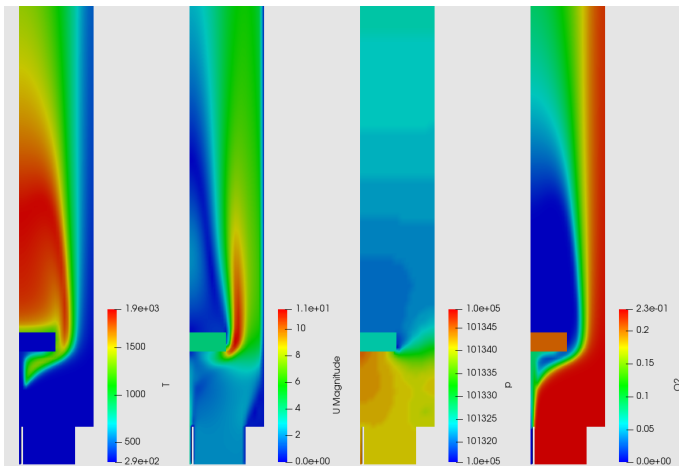
```
./Allrun  
paraFoam &
```

Final solid temperature at $t=0.5s$



Motivation for multiRegionReactingFoam

Some results after $t=0.5s$



Final Slide

Thank you for your time!

Good luck!