Numeric Simulation and Analysis of H_2-O_2 Premixed Combustion Based On Openfoam

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***Abstract*—OpenFOAM is one open source CFD software, reactingFoam is the solver for chemistry and combustion. Cantera is a software tools for problems involving chemical kinetics, thermodynamics,and transport processes. So the coupling of OpenFOAM and Cantera can provide better simulation of combustion than the solver reactingFoam in OpenFOAM. In this context, we couple OpenFOAM and Cantera, and calculate the same H_2-O_2 premixed combustion case with steady solver coupled with Cantera and different transient solvers coupled and not coupled with Cantera. Through the comparison and analysis of different calculations results of the same case, we can see that solvers coupled with Cantera based on OpenFOAM produce more precision result that solver reactingFoam does in deed, and in general, transient solver can reveal more precision trend than steady solver with higher time consumption.**

Keywords-OpenFOAM, Premixed Combustion, Cantera

I. INTRODUCTION

Combustion is a complex chemistry reaction, and it's still a big problem to discribe the whole process accurately[1]. During the combustion process, several phenomena happen meanwhile and affect eath other deeply, such as chemistry reactions, diffusion of heat and species, convective motions induced by the turbulent fluid, and thermodynamics[2].

To avoid the high cost of experimental testing and prototyping, numeric simulation becomes more and more import to understand combustion, especailly turbulent combustion[2]. With numeric simulation, we can understand flame structure and dynamics better to improve existed models.

For now, there are 3 ways for simulation, direct numerical simulations(DNS), Reynolds Averaged Navier-Stokes(RANS) computations and Large-eddy simulations(LES)[2-3]. In general, RANS is the most common way and adopted in this context, too.

For example, micro combustor in micro-power equipments plays a important role, the studies on it have been done with numeric simulations[4]. And some numeric simulating researches have focused on the emission of NOx of combustion or combustion in engine[5-8].

In this context, we introduce the coupling of OpenFOAM and Cantera, then mainly use 3 different solvers including steady and transient ones to simulate the premixed combustion of H_2-O_2 in a 2-dimentional flowfield, after simulations done, we compare the difference among the results generated by diffenrent solvers.

II. OPENFOAM AND CANTRERA

OpenFOAM is an abbreviation for Open Source Field Operation and Manipulation, it's a C++ library indeed[9]. OpenFOAM contians pre-process and post-process tools, sush as meshing tools, paraView for visualization of result. What's more important, OpenFOAM allows user to develop their own new solvers for specific targets based on its standard solvers. That's the key point for us to use OpenFOAM to develop new program to simulate combustion in the context. The whole structure of OpenFOAM is shown in figure 1 as following.

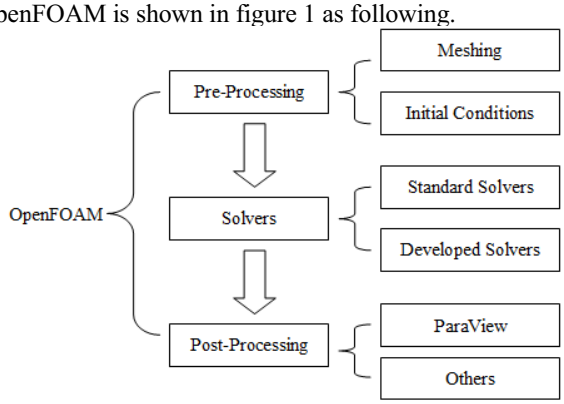

Figure 1. OpenFOAM's Structure

Anyway, in OpenFOAM 1.5.x, there are not so many solvers for combustion, however in later versions, there are fireFoam, chemFoam solvers for chemistry or combustion. But reactingFoam solver remains all the time, so we use this one for comparison in this context.

Cantera is a collection of object-oriented software tools for problems involving chemical kinetics, thermodynamics,and transport processes[10]. It allows C++, Python, Fortran 90 or MATLAB to access its kernel.

For example, with C++, we can access the kernel of Cantera as following[10].

```
include "Cantera.h"
IdealGasMix gas("chem.xml");
gas.setState_TPX(300.0, OneAtm, "CH4:1, O2:2");
```

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cout << "molar enthalpy = ", gas.enthalpy_mole();

This code uses ideal gas for simulation, and reads relative data from a file named “chem.xml”, then sets temperature, pressure and mole fractions state of ideal gas, finally, prints out its molar enthalpy. It’s easy for developer to understand because they don’t need to understand what’s going on inside.

III. COUPLING OF OPENFOAM AND CANTERA

Since Cantera can resolve those problems involving chemical kinetics, thermodynamics,and transport processes, and it’s easy to handle, so Cantera counld be one perfect candidate for the development of solver for chemical reactions.

Gschaider et al. have implemented the coupling of OpenFOAM and Cantera[11]. The solvers they’ve developed are one steady solver and one transient solver. The basis of transient solver is reactingFoam, but the interfaces to Cantera is applied within the new solver.

The steady solver is necessary when simulating large scale chemistry reactions. The implementation of steady solver requires at leat 3 changes as following[11].

(1) SIMPLE algorithm;

(2) Coupling of chemistry to the flow-time;

(3) Stabilization of the solution.

Besides the coupling of OpenFOAM and Cantera, the coupling of ChemApp and OpenFOAM has been implemented successfully[12]. With this kind of coupling, we can get better combustion simulation based on the chemical tool package due to the openness of OpenFOAM.

IV. SIMULATIONS

H2-O2 premixed combustion’s initial conditions are shown in table 1 as following.

In the case, the 2-D mesh is constructed by blockMesh command, shown in figure 2 as following. Notice that the patch type is empty along Z-axis.

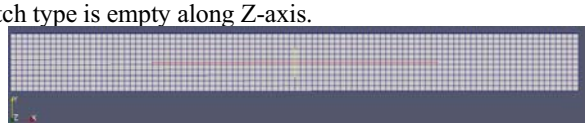

Figure 2. 2-D Mesh

The combustion’s reacting mechanism is from Cantera with 9 species and 27 reactions as following[13].

Elements: O H Ar.

Speicies：H_2 H O O_2 OH H_2O HO_2 H_2O_2 AR.

Reactions are shown in table 3 as following in Cantera format.

The following results will be generated with different solvers based on the same case.

To make better comparison between different simulations, we use the ChemKin ideal gas and ChemApp ideal gas as references to understand which is closer to the ideal gas.

V. RESULTS AND ANALYZE

With 3 different solvers, we simulate the premixed combustion of H_2-O_2, and the average time consumption of transient solvers is shown in table 4 as following.

We can see that with the increment of CPU numbers, the coupled transient solver solves the case faster than the reactingFoam. But we must notice that the sub-parameter named “n” of parameter “simpleCoeffs” in decomposeParDict file. The sub-parameter “n” discribes the distribution of CPUs along XYZ axis. With the same number of CPU, different “n” means different efficiency and time comsumption.

All the plots are done through the X-direction. After simulations, we can get the plots as following.

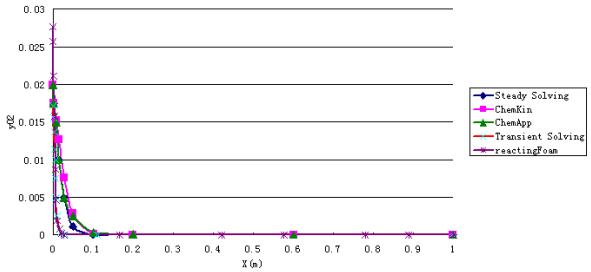

Figure 3. Plot of O2

We can see that all the simulations have the almost same trend, the combustion happens near the inlet immediately, and O2 is used up totally within 0.1 metre along X-direction.

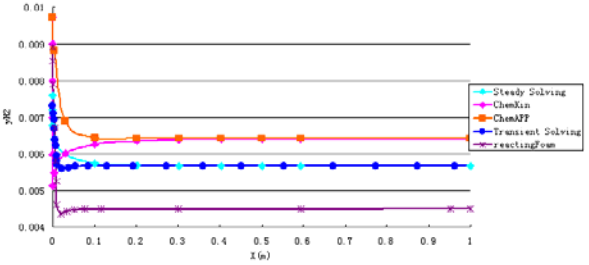

Figure 4. Plot of H2

H2 is consumed sharply along X-direction, but not used up totally.

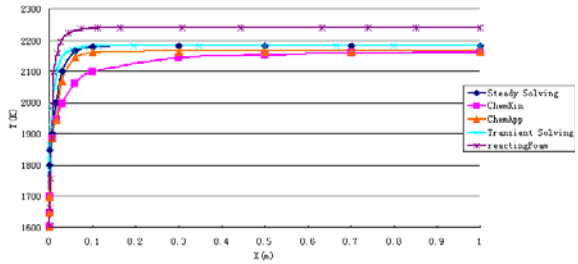

Figure 5. Plot of Temperature

We can see that the temperature varies according different solvers, and the solvers coupled with Cantera reach almost the same temperature as the ideal gas, solvers coupled with Cantera reach 2181K, ChemKin ideal gas reaches 2160K, and ChemApp ideal gas reaches 2164K, the deviation is about 17K~21K, the reason may be the different mechanisms respectly.

But reactionFoam produces a top temperature of 2241K, the deviation is about 77K~81K due to different mechanism.

Anyway, all the simulations show the same behaviors on temperature trend, but solvers coupled with Cantera seem better than reactingFoam.

The ChemKin or ChemApp ideal gas curves are not given in the plots below, but only the curves produces by reactingFoam and solvers coupled with Cantera given because different mechanism means different middle products.

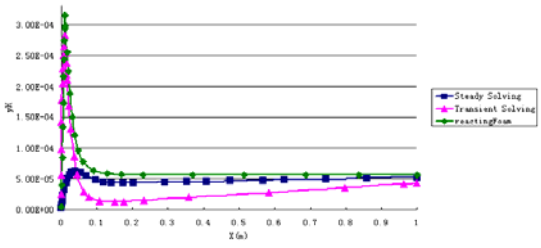

Figure 6. Plot of H

The trend seems the same, but reactingFoam and transient solver coupled with Cantera's behaviors seem closer than that of steady solver.

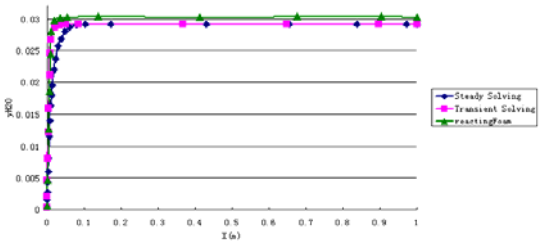

Figure 7. Plot of H_2O

On the genaration of H_2O, different solvers show almost the same behaviors, and again, solvers coupled with Cantera produce the same result, but reactingFoam produces a higher result.

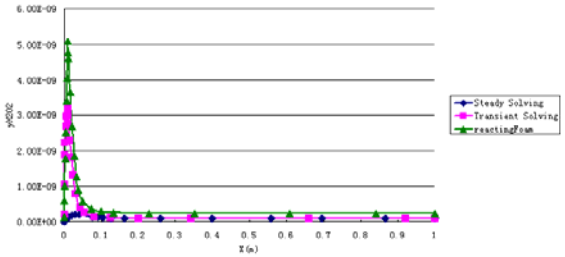

Figure 8. Plot of H_2O_2

All the plots show that the combustion happens near the inlet, and all the final products and middle products reach the peak at the almost same place, then drop or rise to one steady state.

So we can draw somes conclusions from the simulations above.

(1) Transient simulation is more precision than steady one, but much slower than steady one. Transient solvers including reactingFoam and transient solver coupled with Cantera can show the more precision trend due to the difference between SIMPLE and PISO algorithms.

(2) Solvers coupled with Cantera is more precision than reactingFoam solver, especially on temperature, the highest temperature calculated by reactingFoam is about 77K~81K higher than ideal gas's top temperature. We can see that Cantera provides better chemistry mechanism than OpenFOAM itself does.

(3) The coupling of OpenFOAM and Cantera is satisfying. The solvers coupled with Cantera can reach the same result finally, reactingFoam's deviation is within acceptable range.

VI. SUMMARIES

Combustion simulation is more and more important to combustion research, and due to the openness of OpenFOAM, we can couple other tool packages with OpenFOAM besides Cantera, with the coupling, we can get better result of simulation.

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TABLE I. TAB. 1 INITIAL CONDITIONS

Item	Value
Input Velocity	1m/s
Pressure	1bar
Temperature	1600K
Y_{O2}	0.026
Y_{H2}	0.009
Y_{AR}	0.965

TABLE II. TAB.2 MESH SIZE

Orientation	Size	Dimensions
X	1m	100
Y	0.1m	11
Z	0.001m	1

TABLE III. TAB.3 REACTIONS

NO	Reactions	NO	Reactions
1	2 O + M <=> O2 + M	15	H + HO2 <=> O2 + H2
2	O + H + M <=> OH + M	16	H + HO2 <=> 2 OH
3	O + H2 <=> H + OH	17	H + H2O2 <=> HO2 + H2
4	O + HO2 <=> OH + O2	18	H + H2O2 <=> OH + H2O
5	O + H2O2 <=> OH + HO2	19	OH + H2 <=> H + H2O
6	H + 2 O2 <=> HO2 + O2	20	2 OH (+ M) <=> H2O2 (+ M)
7	H + O2 + H2O <=> HO2 + H2O	21	2 OH <=> O + H2O
8	H + O2 + AR <=> HO2 + AR	22	OH + HO2 <=> O2 + H2O
9	H + O2 <=> O + OH	23	OH + HO2 <=> O2 + H2O
10	2 H + M <=> H2 + M	24	OH + HO2 <=> O2 + H2O
11	2 H + H2 <=> 2 H2	25	2 HO2 <=> O2 + H2O2
12	2 H + H2O <=> H2 + H2O	26	2 HO2 <=> O2 + H2O2
13	2 H + H2O <=> H2 + H2O	27	OH + HO2 <=> O2 + H2O
14	H + HO2 <=> O + H2O	-	-

TABLE IV. TAB.4 AVERAGE TIME CONSUMPTION PER STEP OF DIFFERENT TRANSIENT SOLVERS

Solvers	1 CPU	2 CPUs	4 CPUs	8 CPUs	16 CPUs
reactingFoam	1.322s	0.53s	0.491s	0.412s	0.292s
Coupled Transient Solvers	1.547s	0.815s	0.455s	0.374s	0.267s