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## One-dimensional CFD combustion modeling in porous media

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### Abstract

This article present the progress of in-house one-dimensional CFD combustion modeling in porous media development. Local non-equilibrium heat transfer between solid porous-matrix and fluid phase was coupled in both solid and fluid phase energy equation. Considering transport equation are mass, solid phase energy, fluid phase energy and fuel mass fraction. The kinetic rate was controlled by single step Arrhenius law. Current stage of the development is focusing on qualitative phenomena of the coupled heat flow mechanism in solid porous media and fluid phase. The comparison of flame stabilization of conventional gas phase combustion and combustion within inert porous media was carried out. A case study employing a set of simulation parameter in order to test couple stability and point out physical assessment on combustion in inert-porous media. It is revealed that 1.) Temperature of the solid porous matrix is raised up with non-thermal equilibrium along this region. 2.) Fluid and solid temperature are finally in equilibrium 3.) Heat was transfer from solid to fluid at the preheating zone 4.) Heat was transfer from fluid to solid at the reaction zone 5.) Heat conduction in porous media from the reaction zone back to preheating zone act as additional heat recirculation surplus from conventional combustion flame. The couple in stability has initiate at the last control volume which has negative value of fuel mass fraction. The negative value of fuel mass fraction will resulting in non-conservation of fuel in the domain on the next round of coupling process. The fuel check routine is add in the program to detect and correct the negative value of fuel mass fraction. The relaxation value of 0.001 for all conservation equation is need in order to allow couple stabilized until the convergence is achieved.

**Keywords:** Porous media, Combustion, CFD

### 1. Introduction

There are various application of combustion in porous media in engineering discipline. For example, combustion in inert-porous media, catalytic reactor, fixed-bed gasification. They are resemble in terms of physical modeling point of view. The code can be developed on the same platform with some modification on sub-physical model for each application [1].

Modeling of reacting flow in porous media is more complicate work than the conventional reacting flow. More additional of several sources term are need to incorporate in the equations. For example, 1.) Local heat transfer between solid and fluid phase due to thermal non-equilibrium 2.) Thermal radiation of porous solid matrix 3.) Pressure drop due to flow in porous media 4.) Porous surface volatilization 5.) The porous surface heterogeneous reaction, Implement of commercial code on particular case is more difficult due to multi-physics interaction. In addition, the strong non-linear term is resulting in couple stability issues. Therefore, many of the researchers are developing in-house CFD code rather than using the commercial code [1][2][3].

This paper presents the current stage on in-house code development of the CFD combustion in porous media. The model is consider conservation of mass, fuel species, energy in solid porous matrix, energy in fluid pore space. Heat transfer between solid and fluid phase due to local thermal non-equilibrium is modeled via energy source term in separate solid and fluid energy equation. Fuel consumption and heat release

from oxidation is modeled by Arrhenius law. The code is currently develop in one dimension in order to prevent fluid dynamics complication at this stage. Rather than employ the CFD couple algorithm, velocity field can be simply calculate using ideal gas law as the calorific equation of state with one dimensional modeling. One dimensional code is recommended at the early stage of the complex porous media with combustion development [1] [2]. It has more capability of validation and calibration process. The validation on kinetic model and the energy model can be pointed out. Because of the effect of fluid dynamics was cut off. Moreover, couple of highly non-linear term which is prone to instability situation can easily understand.

### 2. Modeling

There are four transport equations taken in to account. The mass transport in fluid pores phase.

$$\frac{d}{dx} \rho \varepsilon u = 0$$

Where  $\rho$  is the density of fluid,  $\varepsilon$  is the porous matrix void fraction and  $u$  is the fluid phase velocity in  $x$  direction.

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Energy transport in fluid pores phase.

$$\rho u c_f \frac{dT_f}{dx} - \frac{d}{dx} \left[ \varepsilon_s k \frac{dT_f}{dx} \right] - \varepsilon \sum h_{f,i}^0 \dot{m}_i + h(T_s - T_f)$$

Where  $T_f$  is the fluid pores temperature,  $T_s$  is the solid porous matrix temperature.  $k$  is air thermal diffusivity,  $h$  is convection coefficient.

Energy transport in solid porous media phase.

$$\frac{d}{dx} \left[ \varepsilon_s k \frac{dT}{dx} \right] + h(T_s - T_f) = 0$$

Fuel species transport.

$$\frac{d}{dx} (\rho \varepsilon u Y_F) = \frac{d}{dx} \left( D_{BIDIF} \frac{dY_F}{dx} \right) + Su$$

Where  $Y_F$  is the fuel mass fraction,  $D_{BIDIF}$  is the binary diffusivity of the fuel and air mixture,  $Su$  is the heat transfer between solid and fluid phase.

The amount of energy transport between gas pores phase and solid porous matrix phase which depends on the different in local temperature field. This term is taken in source term in both fluid and solid energy transport equation

$$Su = h(T_s - T_f)$$

Local fuel consumption rate is calculated by Arrhenius law which depends on local fluid temperature field and the concentration of the fuel species. All constant parameter is taken from propane one-step global combustion kinetic with the assumption of fuel lean mixture. This term is taken in source term of fuel species transport equation.

$$Su = -A \exp(-EA / R_u T) [C_x H_y]^m MW_{fuel}$$

Local heat release is calculated corresponding to Arrhenius law and the heat of combustion of propane. This term is taken in source term of energy transport equation in fluid phase.

$$Su = -A \exp(-EA / R_u T) [C_x H_y]^m MW_{fuel} \Delta H_C$$

Where  $A$  is the pre-exponential factor,  $EA$  is the activation energy,  $R_u$  is the universal gas constant,  $MW_{fuel}$  is the fuel molecular weight,  $\Delta H_C$  is the

heat of combustion,  $m$  is the fuel reaction order and  $[C_x H_y]$  is the fuel concentration.

Local velocity field is calculate by ideal gas law which density is depends on fluid temperature field. For the sake of simplicity, in current stage of development work is consider fluid property as pure air. The assumption is made that the pressure was constant at 1atm for all range of the calculation domain.

$$P = \rho RT$$

### 2.1 Mesh generation

Mesh generation is in one dimensional for 90 centimeters long. The domain was divided into 100,000 equally control volumes. As shows in the figure (1). The code was tested by employ the material property and boundary condition as shows in the table 1

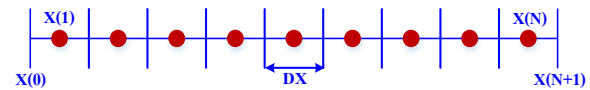


Fig. 1 Mesh generation in calculation domain

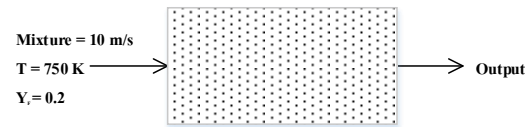


Fig. 2 Boundary condition

Table.1 Boundary condition

Boundary condition	
Mixture inlet velocity	10 m/s
MixtureInlet temperature	750 K
Fuel mass fraction	0.54

Table.2 Material property

Material property	
Porous void fraction	0.5
Fuel molecular weight	0.016 kg/mol
Mixture heat capacity	1000 J/kg.K
Mixturebinary diffusivity	0.0008 m <sup>2</sup> /s
Pressure	101325 N/m <sup>2</sup>
Air thermal diffusivity	100000 W/m.K
Fuel heat of combustion	748310 J/mol
Pre-exponential Factor	1.3x10 <sup>8</sup>
Ea/Ru	24358

All transport equation are discretized into finite volume according to figure 1. In order to calculate convection term, face property was estimate by first order upwind scheme. All transport equation is written

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in system of algebraic equation. Special treatment was executed to boundary mesh according to assigned boundary condition. All of the system of algebraic equations was solved by TDMA algorithm. The equation of state is calculated basis on previous round of solved property field. All of the system of algebraic

equation is then updated. The process is repeated until the convergence criteria is achieved. Relaxation constant and fuel conservation check was added during coupling process otherwise the solution will blow up with highly non-linear term.

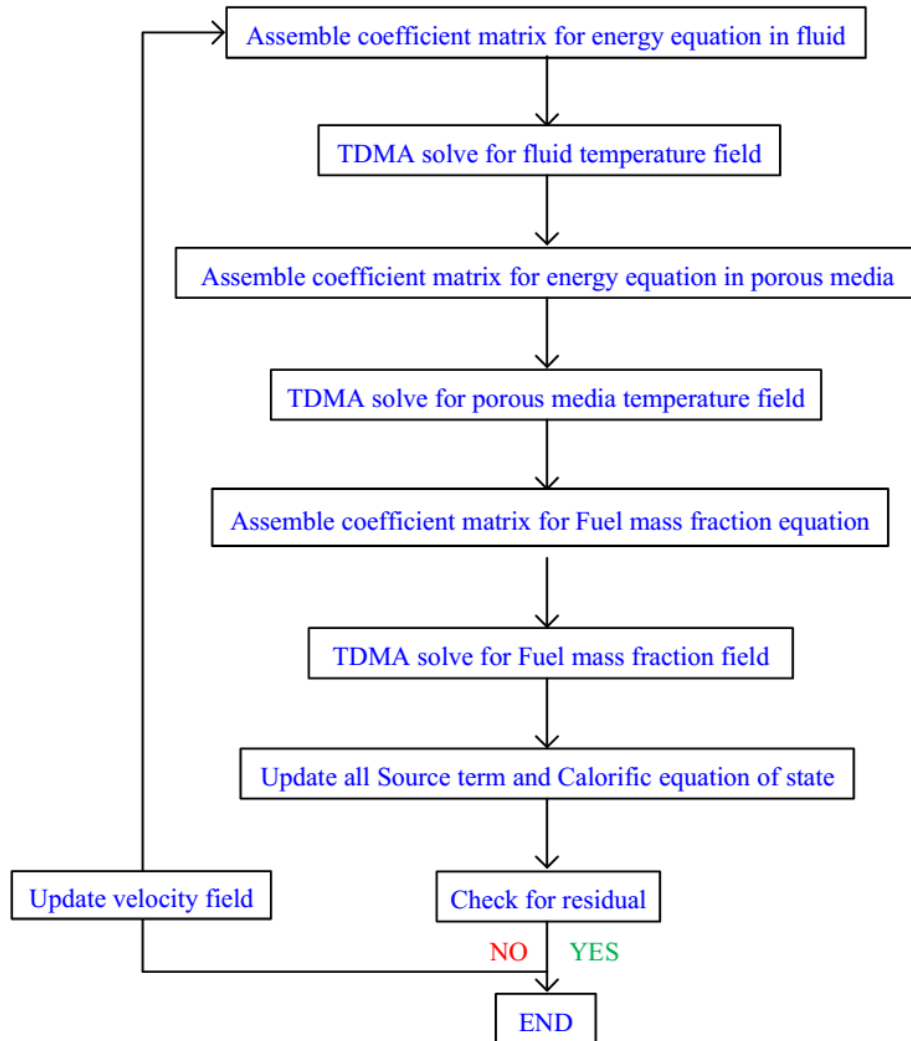


Fig.3 Program flow chart exclude special treatment and relaxation

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### 3. Result and discussion

Gas velocity is accelerated from 15 m/s to 23 m/s during the reaction front as shows in figure 4. Gas temperature is raised due to heat of release from reaction kinetic. Gas temperature is related to gas

density by ideal gas law. Therefore, higher gas temperature is resulting in lower gas density. Regarding to mass conservation equation, with the constant flow cross area, the lower in gas density will increase the flow velocity.

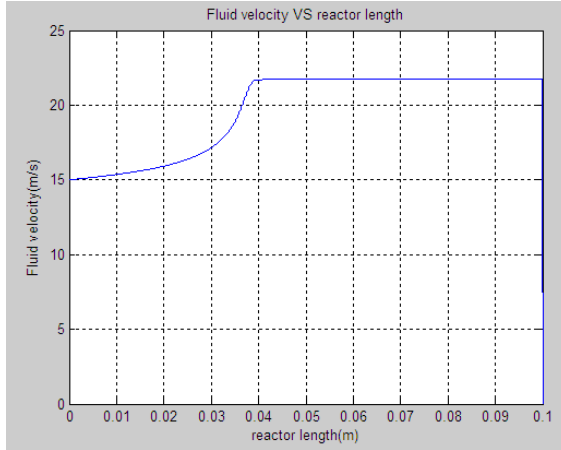


Fig.4 fluid velocity along the combustor length

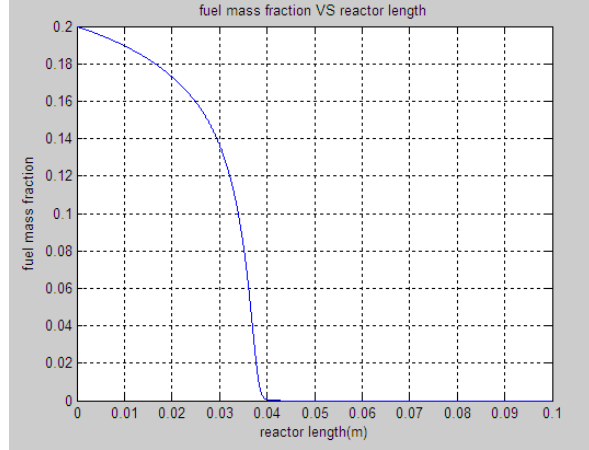


Fig.5 Fuel mass fraction along the combustor length

Fuel consumption and kinetic rate zone is divide into two distinct zone comprising of preheat zone and reaction zone [4]. Preheat zone is dominate by recirculation of the heat released from reaction zone which the diffusion mode of heat and mass transport is appeared. Preheat zone is deliver heat from reaction zone in order to allow continuous on auto ignition process of combustion of fresh cold mixture. The reaction zone is the location where the mixture temperature has reach the level that the fast kinetic rate taking place. The kinetic rate is determine by Arrhenius law which is depends on the exponential of temperature and concentration of the fuel and oxidizer species.

equilibrium zone is restrict around the reaction and preheat zone as figure 7. Solid porous phase promote additional heat recirculation via solid conduction mode. Surplus heat is transport in counter direction to ignite incoming cold mixture.

Demonstration of the temperature non-equilibrium between solid and fluid phase showing non-

Temperature value of solid porous phase is higher than fluid phase at the preheat zone. Therefore, heat is transport from solid to fluid in this region. Conversely at the reaction zone, heat is transport from fluid to solid porous matrix as shows in figure 7. The overall heat transfer mechanism has promote additional heat recirculation which promote flame stabilization capability. This mechanism has claimed that combustion in porous media is cleaner and it has higher flame temperature than conventional combustion.

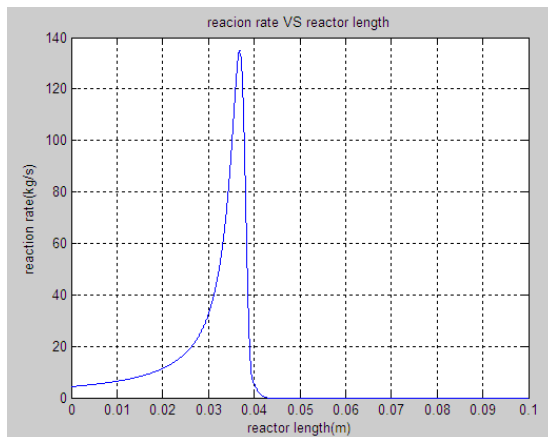


Fig.6 Reaction rate along reactor length

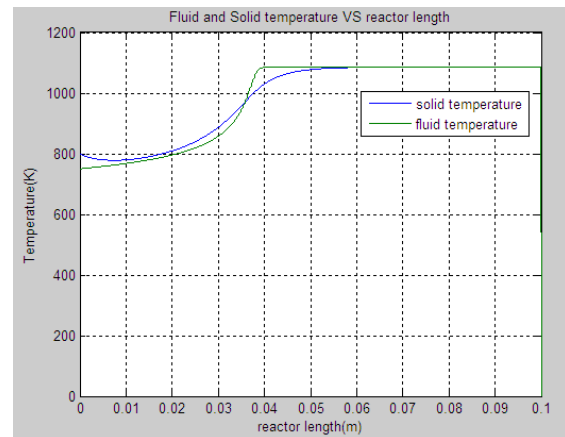


Fig.7 Fluid and solid temperature along reactor length

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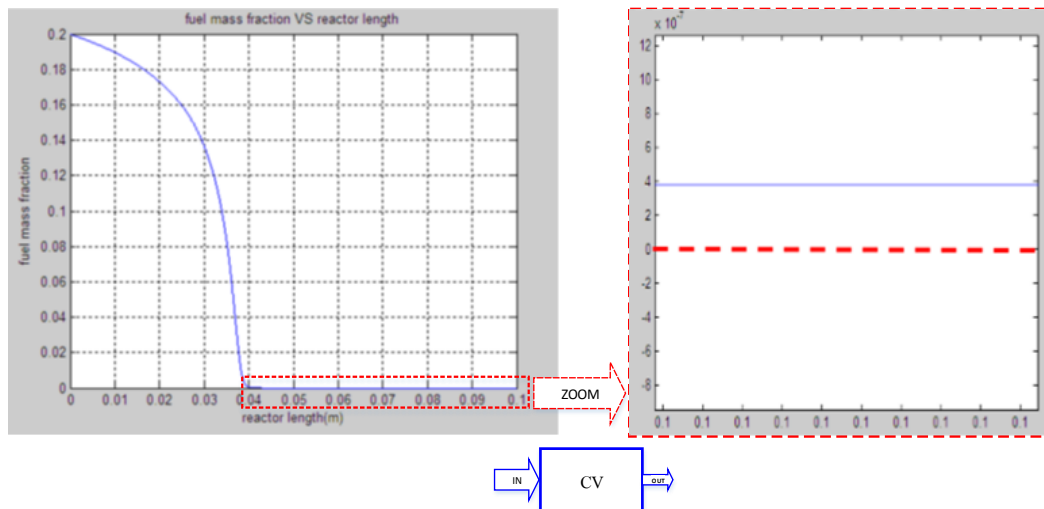


Fig.8 Couple stability because of positive fuel mass fraction along combustor

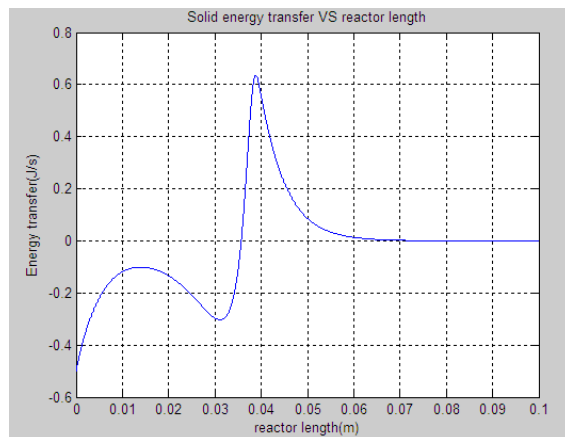


Fig. 9 Solid phase heat transfer

The instability initiate when fuel mass fraction becomes negative value on the last cell. The negative value will resulting in backward fuel transport coming from the end of the combustor. Fuel mass is in violation of conservation from this round of couple because of the additional fuel coming from the end of the combustor. The temperature is raised to infinity by continuing couple for the solution. Therefore, special treatment routine of the program is need in order to ensure that fuel mass fraction is always stay in positive value along the computational domain as shows in figure 8.

#### 4. Conclusion

The comparison of flame stabilization of conventional gas phase combustion and combustion within inert porous media was carried out. It is revealed that 1.) Temperature of the solid porous matrix is raised up with non-thermal equilibrium along this region. 2.) Fluid and solid temperature are finally in equilibrium 3.) Heat was transfer from solid to fluid at the beginning of the reaction 4.) Heat was transfer

from fluid to solid at the end of the reaction. 5.) Heat conduction from the end of the reaction to the beginning of the reaction act as additional heat recirculation from conventional combustion flame. The coupling in stability has initiate at the last control volume which has negative value of fuel mass fraction. The negative value of fuel mass fraction will resulting in non-conservation of fuel in the domain on the next round of coupling process. The fuel check routine is add in the program to detect and correct the negative value of fuel mass fraction. The relaxation value of 0.001 for all conservation equation is need in order to allow couple stabilized until the convergence is achieve

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