SPH Simulation of premixed methane/air combustion in a micro-planar combustor

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1. Introduction

Rapid chemical reactions, such as graphite oxidation and hydrolysis, occur during the VHTR accidents, such as air ingress, due to its high operating temperature. They are known to have devastating effects on the structural integrity of reactor structures and fuel elements [1]. Some safety analysis codes, including GAMMA+, has been developed to predict thermo-fluid and chemical reaction behavior during the accidents.

In this study, gas-phase chemical reaction model is newly developed in SPH framework, and implemented into SOPHIA, which is an SPH-based and GPU-parallelized multi-physics code developed by Seoul National University. In order to validate the model, simulation of methane/air combustion in a planar combustor is carried out, and its results are compared with those of benchmark experiment and simulation. Our simulation gives good agreements with the benchmark results qualitatively and quantitively.

2. SPH methodology

2.1. SPH concept

Smoothed Particle Hydrodynamics (SPH) is a totally Lagrangian computational method for simulating mechanics of continuum media such as a fluid or a solid. In SPH, entire system is represented as a set of particles, which are considered as a continuum, and each particle behaves under the governing equations. As continuum interacts with neighboring continuums by exchanging momentum, energy, etc., SPH particle is affected by its adjacent particles. This interaction is achieved by solving the governing equations in kernel-averaged summation over the neighboring particles which is called the SPH interpolation. Due to its own Lagrangian nature, SPH has various advantages over other Eulerian methodologies in dealing with multi-phase flow, free-surface flow, highly deformable geometry, and so on. Open boundary model has been recently developed for a channel flow, and succeeded in imposing boundary conditions properly, which was once pointed as a defect of SPH [7].

2.2. Chemical reaction model

The Arrhenius equation describes the relation between chemical reaction rate and temperature of components. It is widely used in many engineering fields including nuclear engineering since it is simple and works well in various chemical processes. In SOPHIA, the Arrhenius equation is also utilized to model chemical reactions. Combustion mechanism used in this study is a one-step irreversible reaction proposed by Westbook and Dryer [2] as the below.

$$\dot{R}_{CH_4} = 6.7 \times 10^9 \exp\left(-\frac{202505.6}{RT}\right)[CH_4]^{0.2}[O_2]^{1.3} \quad (1)$$

where $\dot{R}_{CH_4}$ is in units of mol/m^3/s and the concentrations in mol/m^3. This simplified mechanism is known to be a good approximation for explaining flame dynamics, showing quite good agreement with experiments and the detailed reaction mechanism [2]. Five gas species are accompanied: N_2, O_2, CH_4, CO_2, and H_2O. Chen et al. [3] showed that the mechanism gives reasonable agreements with the detailed reaction mechanism, which 16 different gas species and 25 reversible reactions are considered, in the same benchmark problem.

Since according to the gas kinetic theory, chemical reaction occurs when molecules collide with each other (i.e., occurs at a molecular level), the reaction is modeled to occur only within a gas particle. The reaction of each gas particle is affected by molecular diffusion between adjacent particles, not by themselves.

2.3. Governing equations

In this study, mass summation method is used to solve the mass conservation. It is known that simple mass summation leads to over-smoothed density field, resulting in unphysical momentum near sharp density interface [4]. To prevent this, mass summation is reformulated in terms of normalized density as follows.

$$< \rho >_i = \rho_{ref,i} \sum_j \frac{m_j}{\rho_{ref,j}} W_{ij} \quad (2)$$

where ρ_{ref} denotes initial density of a particle.

The multi-component molecular diffusion plays significant role on the combustion process due to its high operating temperature. The species equation with molecular diffusion is formulated by Fick's law as follows.

$$\frac{d}{dt}\rho Y_k = -\rho Y_k \nabla \cdot \vec{u} + \nabla \cdot (\rho D_{k,m} \nabla Y_k) + \dot{R}_k \quad (3)$$

where Y_k, $D_{k,m}$ and $\dot{R}_k$ denotes mass fraction, mass diffusivity, and reaction rate of gas species *k*. The eqn (3) is formulated in SPH manner as the eqn (4).

The pressure and viscous force are considered in the momentum equation (eqn (5)). The equation of the energy conservation, eqn (6) includes enthalpy change of

Table 1. SPH Governing equations and thermodynamic properties

Mass	$< \rho >_i = \rho_{ref,i} \sum_j \frac{m_j}{\rho_{ref,j}} W_{ij}$	(2)
Species	$< \frac{d}{dt}\rho Y_k >_i = Y_k \frac{\rho_i^n - \rho_i^{n-1}}{\Delta t_n} + \sum_j \frac{4\rho_i\rho_j D_{k-m,i} D_{k-m,j}}{\rho_i D_{k-m,i} + \rho_j D_{k-m,j}} \frac{m_j}{\rho_j} \left(Y_{k,i} - Y_{k,j}\right) \frac{\vec{r}_{ij} \cdot \nabla_i W_{ij}}{\left\|\vec{r}_{ij}\right\|^2} + \dot{R}_k$	(4)
Momentum	$< \frac{d\vec{u}}{dt} >_i = \sum_j -m_j \frac{P_i + P_j}{\rho_i \rho_j} \nabla_i W_{ij} + \sum_j \frac{4\mu_i\mu_j}{\mu_i + \mu_j} \frac{m_j}{\rho_i\rho_j} \left(\vec{u}_i - \vec{u}_j\right) \frac{\vec{r}_{ij} \cdot \nabla_i W_{ij}}{\left\|\vec{r}_{ij}\right\|^2}$	(5)
Energy	$< \rho c_P \frac{dT}{dt} >_i + \sum_k \rho h_k \frac{Y_k^n - Y_k^{n-1}}{\Delta t_n}$ $= R_T' + \frac{P_i^n - P_i^{n-1}}{\Delta t_n} + \sum_j \frac{4k_i k_j}{k_i + k_j} \frac{m_j}{\rho_j} \left(T_i - T_j\right) \frac{\vec{r}_{ij} \cdot \nabla_i W_{ij}}{\left\|\vec{r}_{ij}\right\|^2} + \sum_k \sum_j \frac{4\rho_i\rho_j h_{k,i} h_{k,j} D_{k-m,i} D_{k-m,j}}{h_{k,i}\rho_i D_{k-m,i} + h_{k,j}\rho_j D_{k-m,j}} \frac{m_j}{\rho_j} \left(Y_{k,i} - Y_{k,j}\right) \frac{\vec{r}_{ij} \cdot \nabla_i W_{ij}}{\left\|\vec{r}_{ij}\right\|^2}$	(6)
Properties	Mass-fraction weight: $\mu_{mix} = \sum_i Y_i \mu_i$, $c_{P,mix} = \sum_i Y_i c_{P,i}$, $k_{mix} = \sum_i Y_i k_i$	
	Binary diffusivity: $D_{ab} = \frac{0.00266 T^{3/2}}{P \sigma_{ab}^2 M_{ab}^{0.5} \Omega_D}$	Mixture diffusivity: $D_{s-mix} = \frac{1 - f_s}{\sum_{j,j \neq s} (f_j / D_{sj})}$
	Conductivity: $k_i = \frac{15}{4} \frac{R}{M_{w,i}} \mu_i \left[\frac{4}{15} \frac{c_{p,i} M_{w,i}}{R} + \frac{1}{3}\right]$	Viscosity: $\mu_i = 2.669 \times 10^{-6} \frac{(M_i T)^{0.5}}{\sigma_i^2 \Omega_v}$

chemical reactions, pressure change, conduction, and energy transport by molecular diffusion in sequence. Viscous dissipation is disregarded in this study due to its negligible effects.

Pressure of a gas particle is calculated by the ideal gas law as below.

$$P_i = \rho_i R_s T_i \tag{7}$$

where R_s is a specific gas constant. In SPH methodology, Tait's equation is commonly adopted as an equation of state (EOS) for various kind of liquids and gases, and selects artificially low speed of sound for numerical stability. We think it is reasonable that the artificial speed of sound is also employed in the ideal gas law by reducing a specific gas constant as a factor of the below ratio.

$$\frac{R_s'}{R_s} = \left(\frac{u_{max}}{Ma}\right)^2 \left(\frac{1}{\gamma R_s T}\right) \tag{8}$$

where R_s', u_{max} and γ is an artificial specific gas constant, maximum velocity of a gas particle and c_p/c_v, respectively. Mach number, Ma is set to be about 0.1 for incompressibility.

Enthalpy and specific heat of each gas species is calculated by a polynomial fitting of temperature given by NIST, and the kinetic theory is chosen for viscosity, mass diffusivity, and conductivity of each gas species. Enthalpy, heat capacity, viscosity and conductivity of a mixture gas are calculated as a mass fraction-weight average of all gas species, and mixture mass diffusivity is by the kinetic theory [5]. The combustor wall is made of a stainless steel 316 (SS316), and its specific heat, conductivity and density are given by [6].

2.4. Boundary conditions

Open boundary model [7] is employed to simulate a simple planar channel flow in SPH methodology. At the inlet, uniform flat velocity profile is imposed, and mass faction of each gas species is specified, satisfying stoichiometric condition of premixed methane/air mixture combustion. pressure and temperature at the inlet are set to be constant.

SPH pressure-outlet boundary condition is newly developed and employed to satisfy fixed-pressure (1 atm) condition at the outlet. As seen in Fig. 1, pressure field of the outlet is a linear interpolation between pressure of gas particles near the outlet, $P_{f,outlet}$ and atmospheric pressure. The velocity of the particles near the outlet is largely affected by the linear pressure distribution, and as explained in [7], the values of the velocity are assigned to the outlet particles.

When $P_{f,outlet}$ is below a specific value, the outlet particles are a little bit slow down to increase $P_{f,outlet}$ ($u_{outlet} = \beta \frac{\rho_{inlet}}{\rho_{outlet}} u_{inlet}$, $\beta = 0.6 \sim 0.8$). The specific value of 1.02 atm is chosen for a stable flame structure.

No-slip and zero molecular diffusion are employed at the gas-wall interface. At the outer wall surface, convection and radiation heat transfer with the surrounding environment are considered. Convective heat transfer coefficient, h_{conv} and emissivity, ϵ are set to be 15 W/m^2/K and 0.65, respectively.

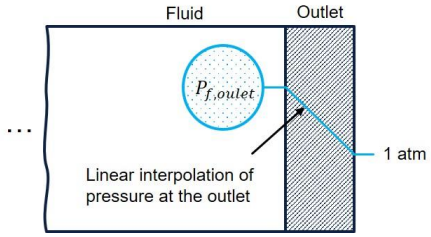

Fig. 1. SPH pressure-outlet boundary

2.5. Particle refinement model

Fresh methane/air mixture injected at the inlet is heated by the hot combustor wall and largely expands its volume, especially near a combustion zone. This leads to increase of inter-particle distance, resulting in low accuracy of SPH interpolation. To address this problem,

particle refinement model [8] is adopted, which splits a voluminous particle into refined (smaller) ones. Particle refinement occurs twice: ① into 4 refined particles when density of a particle decreases less than 0.9 times initial density and ② two new refined particles from the first refined particle when density of the first refined ones reduces less than 0.4 times initial density (Fig. 2). Since error of the refinement are known to be minimized when a refined particle has the same smoothing length of an original one, smoothing length is enforced to be constant despite particles are split and become smaller.

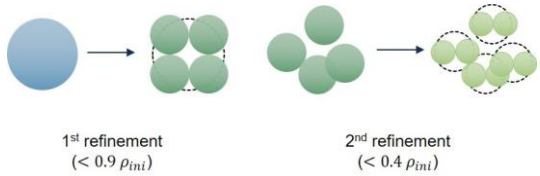

Fig. 2. Particle refinement

2.6. Symmetric boundary model

The combustion phenomenon of the validation problem is totally symmetric about x-axis in both transient and steady states. In our simulation, asymmetric flame structures are observed without any treatments. We think this is due to round-off errors in computing operations on GPU. It seems that the errors are accumulated and amplified at every time-step, finally causing the unphysical asymmetry of combustion flames. Once the asymmetry has occurred, the symmetry is never restored. Symmetric boundary model, which simply mirrors the top half of the system with all flow field variables being symmetrized about x-axis, is newly constructed to correct the errors. The mirroring is performed in every 800-2000 counts which is found to be enough to give perfect symmetry in our simulation with negligible computational loads.

2.8. Time integration

In SOPHIA, governing equations are explicitly time-integrated by a modified predictor-corrector algorithm [4]. In the case of rapid chemical reactions like combustion, it seems better to apply simple Euler method rather than the predictor-corrector method since the predicted value of gas concentration can make the mass conservation unsatisfied. Therefore, time integration on the species equation is carried out with the Euler method, and others with the predictor-corrector method.

In this study, time-step is simply determined by particle acceleration and reaction rate, and formulated as below.

$$\Delta t = min\left(0.1\sqrt{\frac{h_i}{a_i}}, 0.1\frac{[O_2]_i}{\left(\frac{d[O_2]}{dt}\right)_i}, \Delta t_{min}\right) \qquad (9)$$

where h_i and a_i are smoothing length and acceleration of particle i. Δt_{min} denotes specified time-step by a user, which has an order of magnitude of 10^{-6} [s].

3. Simulation of 2D micro-combustor

3.1. Simulation setup

In this study, simulation and experimental results of a micro-planar combustor by Tang et al. are selected as benchmark data for the model validation. As illustrated in Fig. 1., the configuration is a rectangular channel with the height 3 mm and the horizontal length 18 mm. The wall thickness is 0.5 mm, so the height of straight channel is 3 mm. Premixed mixture of methane/air gas is flowing into the inlet with uniform velocity profile (0.4 m/s) during the operation process. The gas mixture, of which temperature is initially 300 K, is heated by the hot wall, and is combusted near the reaction zone inside the combustor. The burned gas is cooled down flowing along the channel and comes out of the outlet. The combustion is stoichiometric.

A homogeneous flow field with the same conditions at the inlet is shortly ignited for the initialization of the simulations which is imperative to burn the fuel. Therefore, a spatial heat source term with an ignition strength 5.0e+9 J/m^3 is additionally included in the equation of the energy conservation for 1.5e-4 s. Initial temperature of the combustor wall is set similar to wall temperature distribution of Tang et al.

Initially, about 8,000 SPH particles are participated in the simulations, but due to the particle refinement, the number of the participated particles reaches about 20,000.

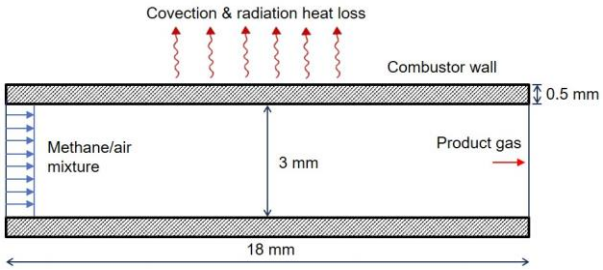

Fig. 3. Simulation geometry

3.2. Simulation results

Fig. 3 shows comparison of the flame structures by SOPHIA and Tang et al. Similar flame structures are observed, but since the different kinetic models are employed for both two results, there are some discrepancy. The locations of the flames are nearly same each other, which implies the similar wall temperature distribution as shown in Fig 4. Since our simulation is totally Lagrangian, the flame is not spatially fixed, slightly changing its location. Specifically, the flame tends to be blown out of the exit without any treatments. Howerever, this tendency is prevented by the pressure-outlet boundary condition explained above. Thanks to

the condition, the flame, which flows downstream slightly due to the tendency, restores its original location. This oscillatory behavior is repeated within very limited region of the planar combustor during total simulation time, but its impact on the wall temperature distribution is negligible.

4. Summary

In this study, the premixed methane/air combustion in the micro planar combustor is simulated with GPU-parallelized SPH solver, SOPHIA. SPH chemical reaction and multi-component diffusion models are newly developed and implemented into SOPHIA for the simulations. The particle refinement model, and the symmetric boundary model are additionally applied in the simulations to satisfy the symmetric condition and enhance the accuracy of SPH interpolation. The SPH open boundary model is adopted to appropriately impose inlet/outlet boundary conditions. The results of SOPHIA give quite reasonable agreements with the benchmark when it comes to the flame structures and the wall temperature distribution.

Acknowledgement

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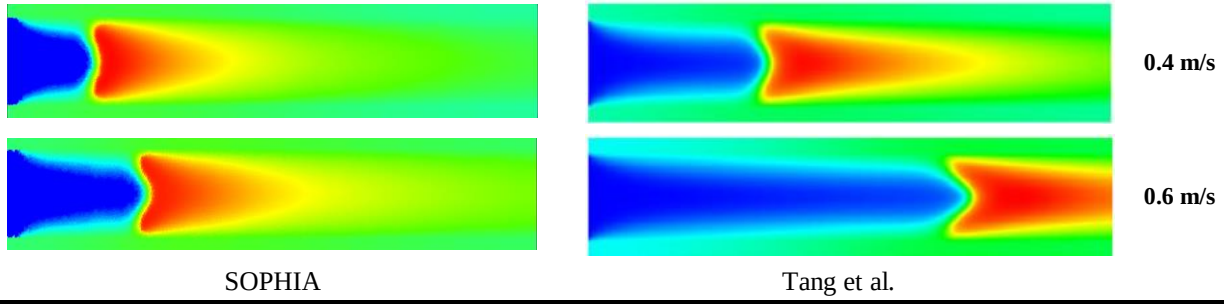

Fig. 4. Flame structures

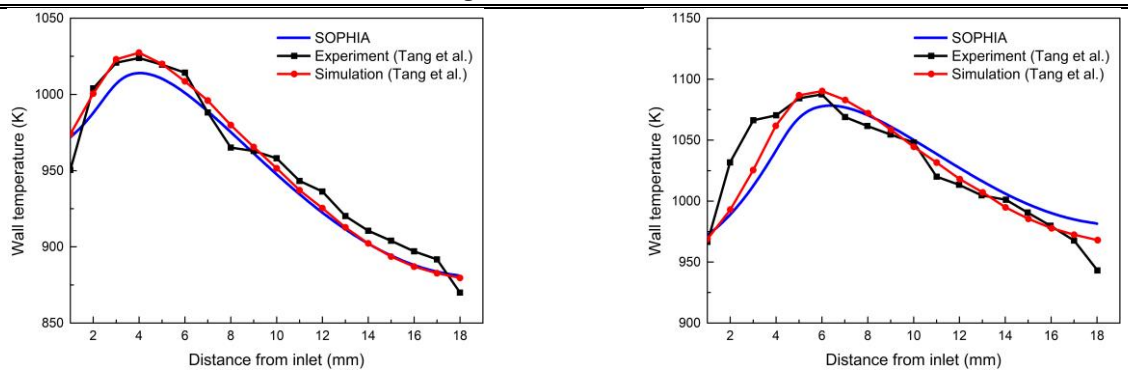

Fig. 5 Wall temperature distribution