Supplementary Material for “Initiation and propagation of spherical premixed flames with inert solid particles”

Submitted to *Combustion Theory and Modeling*

Qiang Li1, Chaoyi Liu2, Huangwei Zhang1, Mengze Wang2 and Zheng Chen2

1 Department of Mechanical Engineering, Faculty of Engineering, National University of Singapore, 117575, Singapore

2 SKLTCS, CAPT, BIC-ESAT, College of Engineering, Peking University, Beijing 100871, China

This supplemental document presents the detailed governing equations of inert solid particle phase in Eulerian framework, which are solved for Section 5 of the manuscript, as well as the detailed derivation procedures for Section 2.

**S1. Governing equations of particle phase in Eulerian framework:**

In the current work, the Eulerian framework is introduced into the A-SURF code [1, 2] and applied to describe the inert particle dispersed in continuous gas phase. The particle phase is treated as an inter-penetrating continuum governed by Eulerian transport equations for number density (i.e. Eq. 1), momentum (Eq. 2) and energy (Eq. 6).

The particle is assumed to be spherical, and the temperature within each particle is assumed to be uniform. The particle-particle interactions and therefore the resultant particle-related diffusion is neglected due to the dilute particle loading in our work. The movement of the particles is affected only by the drag force, without any external body forces (e.g. gravity).

Below we present the governing equations of dispersed particle phase for number density, momentum, and energy in the Eulerian framework and one-dimensional spherical coordinate system.

* **Particle number density**

The evolution of the particle number density read [3]

, (S1)

where is the particle velocity.

* **Momentum conservation**

The motion of particle is determined by Newton’s second law, considering the drag forces resulting from velocity slip between the two phases, and is governed by

, (S2)

where is the velocity of the particles phase, is the drag force applied to a single particle, is the mass of a single particle, is the velocity of gas phase, and is the particle relaxation time expressed as

, (S3)

where and are the density and diameter of the particle, is the dynamic viscosity of local gas phase, is the drag coefficient, and is the particle Reynolds number. In particular, Re is defined as

, (S4)

where is the density of gas phase. has the following relation with Re [4]

. (S5)

* **Energy conservation**

For the energy conservation of particles, we only consider heat transfer between the gas phase and particle phase, heat radiation is neglected. So the energy equation can be written as

, (S6)

where *CP* is the heat capacity of the particle, is the temperature of particle, is the convective heat transfer coefficient, is the surface area of the particle, and is the temperature of gas phase.

The heat transfer coefficient can be estimated using the correlation of Rans and Marshall model [5]. The Nusselt number is calculated as

, (S7)

where is the thermal conductivity of gas phase, is the Prandtl number of the gas phase, and , is the heat capacity of gas phase. From the Nusselt number, we can get the convection heat transfer coefficient

. (S8)

* **Coupling between gas phase and particle phase**

Bi-directional interactions between gas phase and particle phase are included in this work, which have been schematically demonstrated in Fig. 1. The effects of the particle phase on gas phase are considered through adding the following source/sink terms to the right hand side of the corresponding equations of momentum and energy for gas phase [1, 2].

The term for the gas phase momentum equation (the momentum exchange resulting from the mass transfer is not considered here) is

. (S9)

For energy exchange, it takes the following form

. (S10)

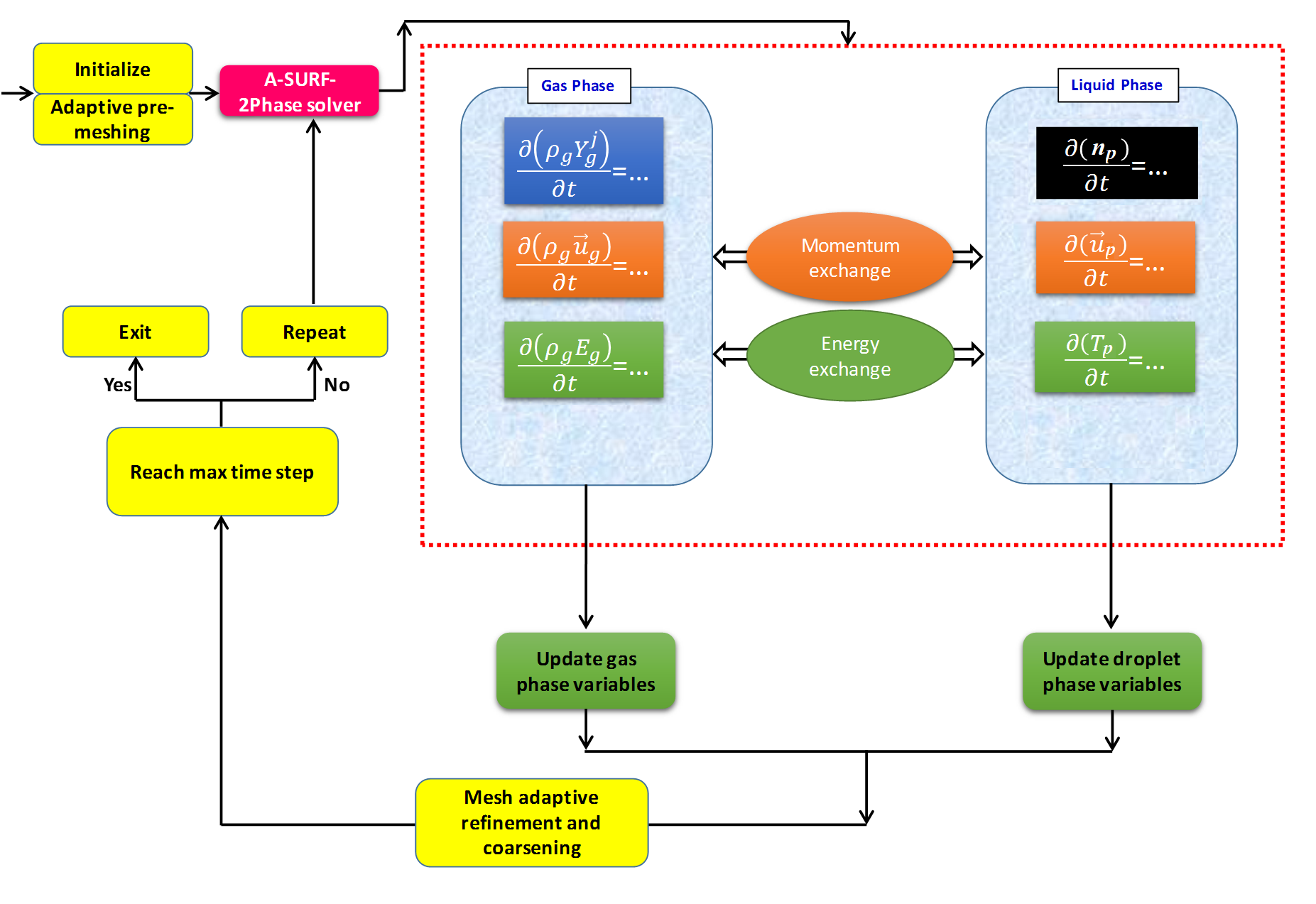
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Figure 1. Flow chart of the A-SURF-2Phase Solver. The procedures within the red dashed box indicate the gas and particle phase solvers and their interactions.

**References**

[1] Z. Chen, M.P. Burke, Y. Ju, Proc. Combust. Inst. 32 (2009) 1253–1260.

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**S2. Derivations of analytical solutions of gas and particle phases**

The governing equations (on Page 11 and 12 of the revision) written with the coordinate system attached to the flame front are

, (S11)

, (S12)

, (S13)

. (S14)

At the flame front (*η* = 0), the following jump conditions hold

(S15)

(S16)

The subscript “0+” denotes the quantities at the unburned size of the flame front, while “0‒” denotes the quantities at the burned side. Here Eqs. (S11) ‒ (S16) are the same as Eqs. (30) ‒ (35) as in the manuscripts.

1. **Particle phase temperature**

Through substituting Eq. (S14) into Eq. (S11), we can eliminate the gas temperature term in Eq. (S11) to obtain the third-order ODE about the particle temperature as

(S17)

Instead of solving the particle temperature directly, we choose to firstly solve . Thus, this third-order ODE about can be-written as a second-order ODE about , i.e.

. (S18)

Here *D1* and *D2* are the integral constants. and is the first derivatives of and . and take the following form

(S19)

(S20)

where

, (S21)

, (S22)

. (S23)

Then the analytical expression for particle temperature can be achieved through integrating Eq. (S18), i.e.

. (S24)

where *D1*, *D2*, and *D3* are the constants which can be determined by the boundary and jump conditions.

Substituting Eq. (S24) into Eq. (S14), we can get the analytical expression of *Tg* as

. (S25)

Table S1 summarize the boundary conditions and jump conditions at the flame front ( =0). The boundary conditions consist of 6 different equations, which can be used to solve the two different sets of *D1, D2*, and *D3* for the unburned zone and burned zone.

Table S1. Boundary and jump conditions for temperature

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | Burned zone  ( | | Unburned zone ( | |
| boundary |  |  |  |  |
| *Tg* |  |  |  |  |
| *Tp* | - |  | |  |
| Jump condition for *Tg* at the flame front |  |  | |  |

Hence, we can obtain the expressions of the three integral constants in the unburned zone and burned zone as. Specifically, for the unburned zone (), they are

. (S26)

For the burned zone (), these integral constants are

,

,

. (S27)

After substituting the Eqs. (S26) and (S27) into Eq. (S24), we can obtain the expression of as

, (S28)

where and are the constants with the following expressions

, (S29)

. (S30)

Equation (S28) corresponds to Eq. (36) in the revised manuscript, whilst Eqs. (S29) and (S30) to Eqs. (38) and (39).

1. **Gas phase temperature**

Substituting the Eqs. (S26) and (S27) into Eq. (S25), one can obtain the expression of as

,

(S31)

where and is the same as Eqs. (S29) and (S30).

1. **Fuel or oxidizer mass fraction**

For the fuel or oxidizer mass fraction, the governing equation (S12) and (S13) can be re-written as

. (S32)

The general solution of Eq. (S32) is

, (S33)

where and are the constants determined by the boundary conditions and jumping conditions for the fuel or oxidizer mass fraction.

The boundary conditions for at the boundaries are tabulated in Table S2

Table S2. Boundary and jump conditions for mass fraction

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | Burned zone  ( | | Unburned zone ( | |
| boundary |  |  |  |  |
| *Y* |  |  | |  |
| Jump condition for *Y* at the flame front |  |  | |  |

Hence, we can get the two integral constants in the unburned zone and burned zone using the conditions in Table S2. Specifically, for the unburned zone (), they are

. (S34)

For the burned zone (), these integral constants are

(S35)

Therefore, the analytical solution for fuel or oxidizer mass fraction distribution is

(S36)

Equation (S36) corresponds to Eq. (45) in the manuscript.

1. **Correlation between flame propagation speed and flame radius**

From the above, we have obtained the analytical solution of the gas temperature , particle temperature and the fuel or oxidizer mass fraction . Through substituting the three solutions into the flame front jump condition (Eq. S16), the correlation between the flame propagation speed, flame temperature and radius can be achieved

(S37)

This is Eq. (46) in the manuscript.