Fully resolved simulation of char particle combustion by IB-LBM

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Fully resolved simulation of char particle combustion by IB-LBM

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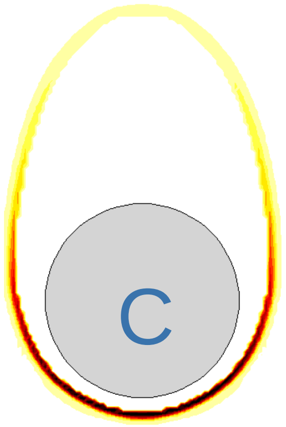

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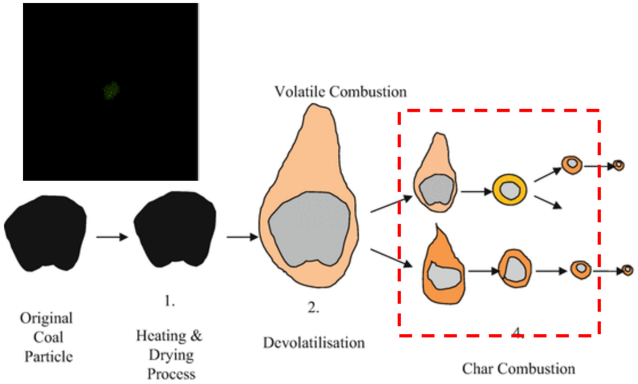
1. Motivation

- Low carbon footprint technologies: Oxy-fuel combustion, Pressurized oxy-fuel combustion, chemical looping combustion…..

- Char combustion: core of coal combustion

  Char combustion time: t_{cc}=3~5 s

  Volatile combustion time: t_{vc}=0.01~0.1 s

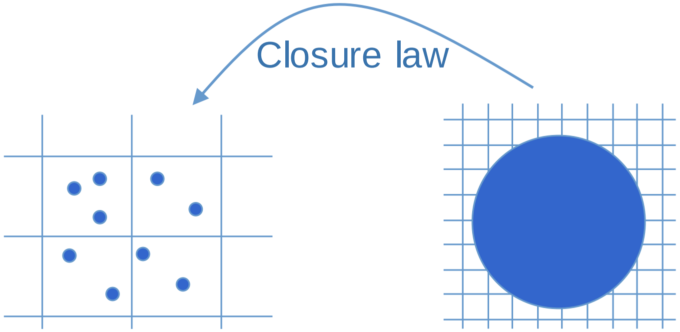


Coal combustion process

- Conventional simulation: 1-D model, particle point (PP) model

  → large error

- FR-DNS: most accurate than 1-D model, build new closure laws for PP model

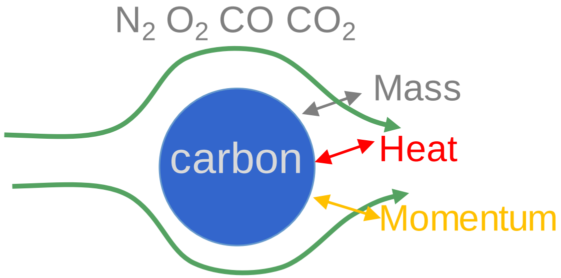


Particle point model Particle resolved model

Most FR-DNS works based on incompressibility hypothesis or non-reactive flows

2 Numerical method

2.1 Assumptions and simplifications



- Burning process is quasi-steady,
- Particle porosity inside particle is neglected,
- Particle consists of carbon only,
- Gaseous environment only consists of N_2, O_2, CO, CO_2,
- Temperature gradient within particle is neglected,
- Water vapor is taken into account by having an effect on the CO oxidation reaction,
- Gas radiation is not taken into account

⬇

Chemical reactions only happen at or outside solid-gas interface

Makino, A, Toshikazu N, Katsuya K. Combustion rates of graphite rods in the forward stagnation field with high-temperature airflow. *Combustion and flame* 2003, 132(4): 743-753.

Luo K, Mao C, Fan J, et al. Fully resolved simulations of single char particle combustion using a ghost-cell immersed boundary method[J]. *AIChE Journal*, 2018, 64(7): 2851-2863.

2.2 CMDF-LBM for low-Mach reactive flows

- Reaction
  - **Heat** produce/consumption
  - **M**ass produce/consumption
- *dT* and d*Y* is large around particle surface

Significant

density fluctuations

$(\rho_{max}-\rho_{min})/\rho_{ave} > 50\%$

Conventional LBM model (Qian, He-Luo…) by incompressible hypothesis ***is improper***

$(\rho_{max}-\rho_{min})/\rho_{ave} < 5\%$

$$\rho = P/c_s$$

- Most industrial flows occur at **low Mach number**:

$$Ma = \frac{u}{c_s} \ll 1$$

Non-linear

Weakly compressible control equations

$$\frac{\partial \rho}{\partial t} + \nabla \rho u = 0$$

$$\frac{\partial u}{\partial t} + u \cdot \nabla u = -\nabla P + \frac{1}{\mathrm{Re}} \nabla^2 u + f$$

$$\frac{\partial T}{\partial t} + u \cdot \nabla T = \frac{1}{\mathrm{Re}\,\mathrm{Pr}} \nabla^2 T + h$$

$$\frac{\partial Y_i}{\partial t} + u \cdot \nabla Y_i = \frac{1}{\mathrm{Re}\,Sc} \nabla^2 Y_i + \omega_i$$

$$P = \rho R T$$

Non-linear

*CMDF-**LBM***

2.2 CMDF-LBM for low-Mach reactive flows

- Coupled Multi distribution function (CMDF) method
- By Chapman-Enskog procedure, weakly compressible control equations can be derived from the followed evolving equations.

Fluid flow

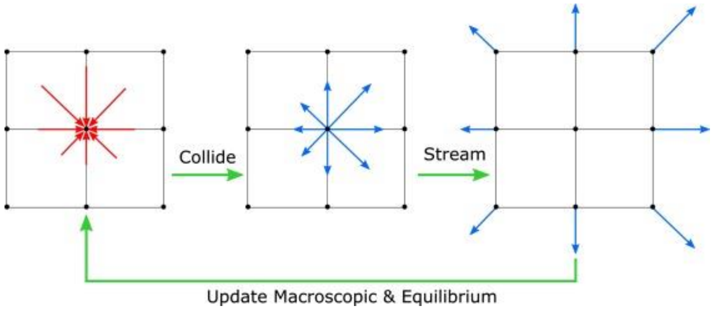
Linear

$$f_i(\vec{x}+\vec{c}_i\Delta t, t+\Delta t) = f_i(\vec{x},t) - \frac{1}{\tau_u}[f_i(\vec{x},t) - f_i^{(eq)}(\vec{x},t)] + \Delta t F_i(\vec{x},t)$$

$$f_i^{(eq)} = \chi_i + \rho\omega_i\left(\frac{(\vec{c}_i\cdot u)}{c_s^2} + \frac{(\vec{c}_i\cdot u)^2}{2c_s^4} - \frac{|u|^2}{2c_s^2}\right) \quad \begin{cases} \chi_0 = \rho - (\omega_0 - 1)\,p/c_s^2 \\ \chi_i = \omega_i\, p/c_s^2 \quad (i \neq 0) \end{cases}$$

$$\boxed{\rho = \frac{p_0\bar{W}}{R_g T} \Rightarrow \rho = \rho_0\frac{T_0 C_0}{T C_{mix}} = \rho_0\frac{T_0\sum Y_{i0}/W_i}{T\sum Y_i/W_i}}$$

$$u = \frac{1}{\rho}\sum_i c_i f_i + \frac{\Delta t}{2\rho}\mathbf{f}_{\text{ext}} \qquad F_i = \left(1 - \frac{1}{2\tau}\right)\omega_i\left(\frac{\vec{c}_i - u}{c_s^2} + \frac{\vec{c}_i\cdot u}{c_s^4}\vec{c}_i\right)\mathbf{f}_{ext}$$



Main steps of LBM (D2Q9)

It will become incompressible for isothermal and nonreactive flows.

Linear

Heat and mass transfer

$$g_{s,i}(\vec{x}+\vec{c}_i\Delta t, t+\Delta t) = g_{s,i}(\vec{x},t) - \frac{1}{\tau_T}[g_{s,i}(\vec{x},t) - g_{s,i}^{(eq)}(\vec{x},t)] + \Delta t Q_{s,i}(\vec{x},t) \quad (s = T, Y_k)$$

$$g_i^{(eq)} = T\omega_i\left(1 + \frac{(\vec{c}_i\cdot u)}{c_s^2} + \frac{(\vec{c}_i\cdot u)^2}{2c_s^4} - \frac{|u|^2}{2c_s^2}\right)$$

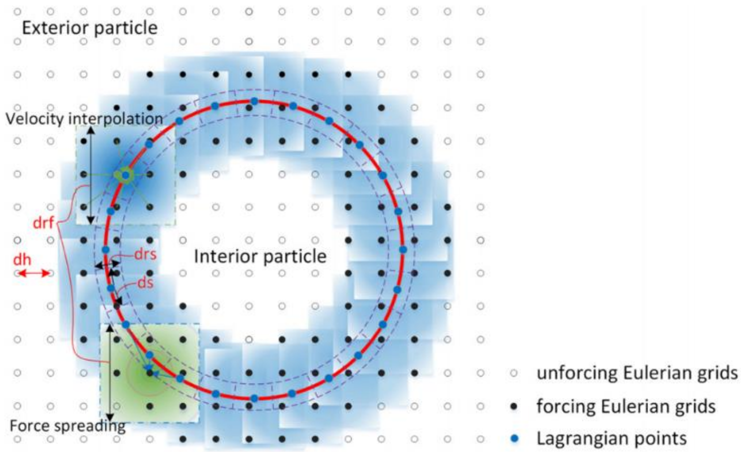
Reaction source

IBM source

$$T = \sum_i g_{T,i} \qquad Y_k = \sum_i Y_{k,i} \qquad Q_i = \omega_i\left(q_r + q_{IB}\right)$$

2.3 BTDF-IBM for reactive gas-solid interaction

- Boundary-Thickening based Direct forcing-immersed boundary method



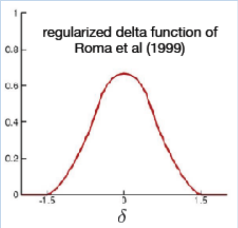
$$F_i = \sum_j^n D_{ik} D_{kj} \varepsilon_j F_j \quad \varepsilon_j = \sum_i \left(D_{ik} D_{kj} \right)^{-1} \quad t = \frac{1}{n} \sum \varepsilon_i \quad f_k = \sum_i D_{ik} t \left(\rho \frac{U_i - \sum_k D_{ik} u^*}{\Delta t / 2} \right)$$

BTDF-IB-LBM

➢ Interpolation and extrapolation operations of IBM

$$D_I = \frac{1}{dh^2} \delta\left(\frac{x-X}{dh} \right) \delta\left(\frac{y-Y}{dh} \right) \cdot dh^2$$

$$D_E = \frac{1}{dh^2} \delta\left(\frac{x-X}{dh} \right) \delta\left(\frac{y-Y}{dh} \right) \cdot \left(drsdh \right)$$

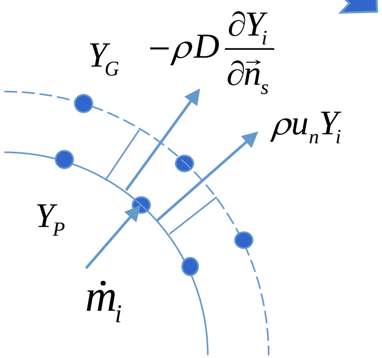


➢ Physical boundary condition

$$u_{stefan} = -\frac{1}{\rho} \dot{m}_C$$

$$\dot{m}_i = -\rho D \frac{\partial Y_i}{\partial \vec{n}_s} + \rho u_n Y_i$$

$$V c_{p,C} \frac{dT_p}{dt} = \int_{surf} \left(-\sigma\varepsilon \left(T_p^4 - T_0^4 \right) + \sum_k M_c R_k \Delta h_k + \left(\lambda \nabla T \right)_s \cdot \vec{n}_s \right)$$



Burning carbon surface

➢ Source terms

$$F_b = 2\rho \frac{u_{stefan} - D_I u^*}{\Delta t}$$

$$f = D_E F_b$$

$$Q_{b,T} = 2 \frac{T_p - D_I T^*}{\Delta t}$$

$$q_{IB,T} = D_E Q_{b,T}$$

$$q_{IB,Y_i} = D_E \frac{\dot{m}_i ds}{\rho dh^2}$$

(Jiang&Liu, *J. Comput. Phys.* , 2019)

2.4 Major reactions of carbon combustion

Heterogeneous reactions

$2C+O_2 \rightarrow 2CO$ (R1)

$C+CO_2 \rightarrow 2CO$ (R2)

Homogeneous reaction

$CO+0.5O_2 \rightarrow 2CO_2$ (R3)

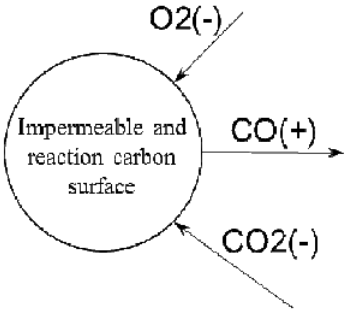
Surface mass produce and consumption

$$\dot{m}_{O_2} = -M_{O_2} R_1 \qquad (\mathrm{kg/m^2s})$$

$$\dot{m}_{CO_2} = -M_{CO_2} R_2$$

$$\dot{m}_{CO} = 2M_{CO}\left(R_1 + R_2\right)$$

$$\dot{m}_{C} = -M_{C}\left(2R_1 + R_2\right)$$

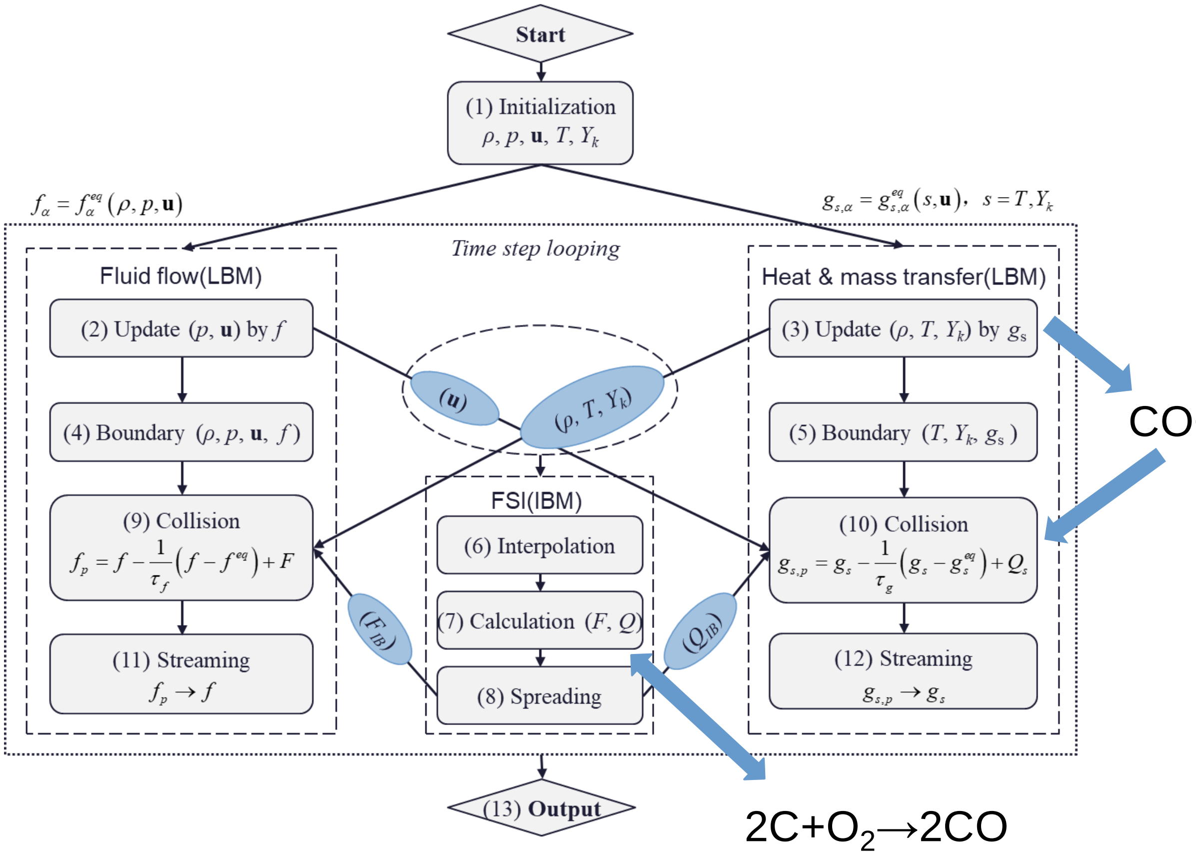


Source term

$$\begin{cases} q_{Y,i} = \dfrac{1}{\rho} R_3 M_i & (1/\mathrm{s}) \\[2ex] q_T = \dfrac{1}{\rho c_p} R_3 \Delta h_3 & (\mathrm{K/s}) \end{cases}$$

Reaction	Reaction rate		Arrhenius formula	Reaction heat Δh, (KJ/mol)
R_1	K_1[O2]	mol/(m^2.s)	K_1=1.97x10^{7}e$^{(-23815/T)}$	221
R_2	K_2[CO2]	mol/(m^3.s)	K_2=1.291x10^{5}e$^{(-22976/T)}$	-173
R_3	K_3[CO] [O2]$^{0.5}$	mol/(m^3.s)	K_2=1.3x10^{8}e$^{(-15094/T)}$	283

Summary of the present IB-LBM method



$CO + 0.5O_2 \rightarrow 2CO_2$

$2C + O_2 \rightarrow 2CO$

$C + CO_2 \rightarrow 2CO$

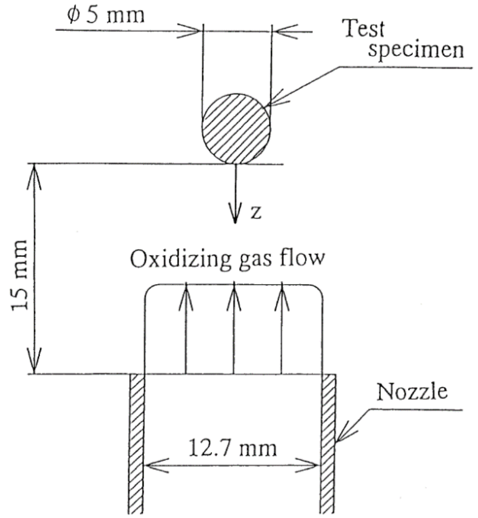
- Density is updated from the equation of state:

$$\rho = \frac{p_0 \overline{W}}{RT} = \frac{\rho_0 T_0 \sum Y_{0,i} / W_i}{T \sum Y_i / W_i}$$

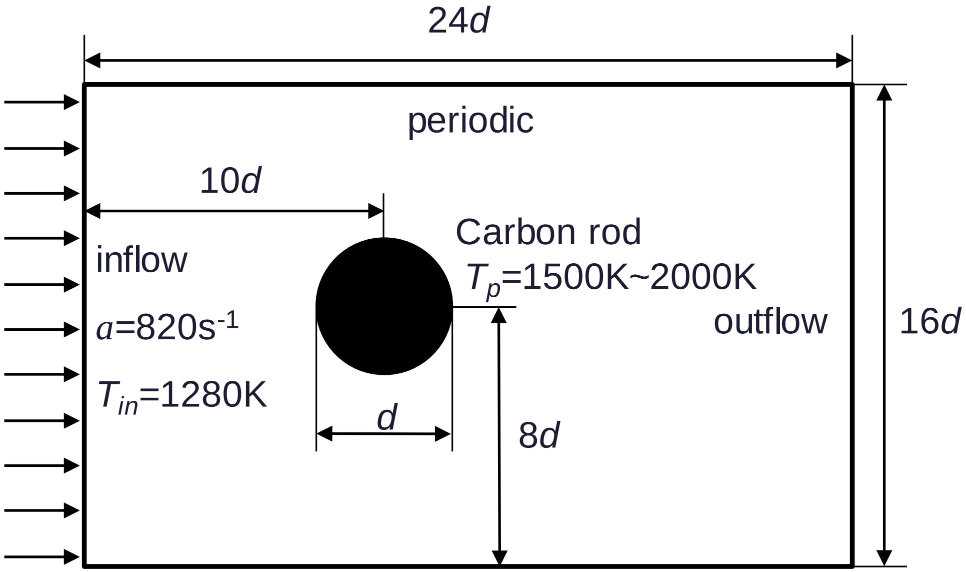
Present IB-LBM method are fully coupled for gas-solid combustion.

2.5 Computation Setup

- Hot air flow past an reactive char particle with constant surface temperature.



Experiment(Makino, 2003)



Present computation domain

Computing parameters

u=1.025 m/s Re ≈ 28

T_p=1500 ~ 2000 K

$\Delta t = 5\times10^{-7}$ s $\Delta x = \dfrac{D_p}{50} = 1\times10^{-4}$ m

$Y_{in,O_2} = 0.233$ $Y_{in,N_2} = 0.767$

Transport parameters

$$c_p = R\left(a + bT + cT^2 + dT^3 + eT^4\right)$$

$$\mu = \mu_0 (a/b)(T/T_0)^{1.5} \qquad \lambda = a(T/T_0)^b \qquad \alpha = \frac{\lambda}{\rho C_p}$$

$$D_{ij} = \frac{0.0266T^{1.5}}{PM_{ij}^{0.5}\sigma_{ij}^2\Omega_D} \qquad D_i = \frac{1-\chi_i}{\sum_{j\neq i}\left(\chi_i / D_{ij}\right)}$$

$$\tau = 0.5 + \frac{\nu}{c_s^2\Delta t}$$

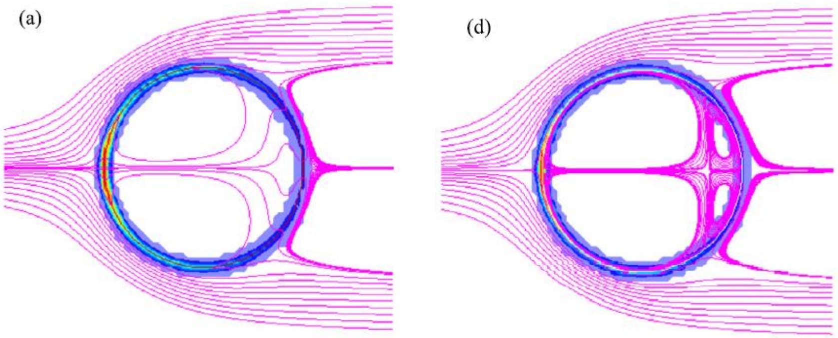
$$\tau_T = 0.5 + \frac{\alpha}{c_s^2\Delta t}$$

$$\tau_{Y_i} = 0.5 + \frac{D_i}{c_s^2\Delta t}$$

Makino, A, Toshikazu N, Katsuya K. Combustion rates of graphite rods in the forward stagnation field with high-temperature airflow. *Combustion and flame* 2003, 132(4): 743-753.

3. Results and discussions

- Validation under non-reaction.

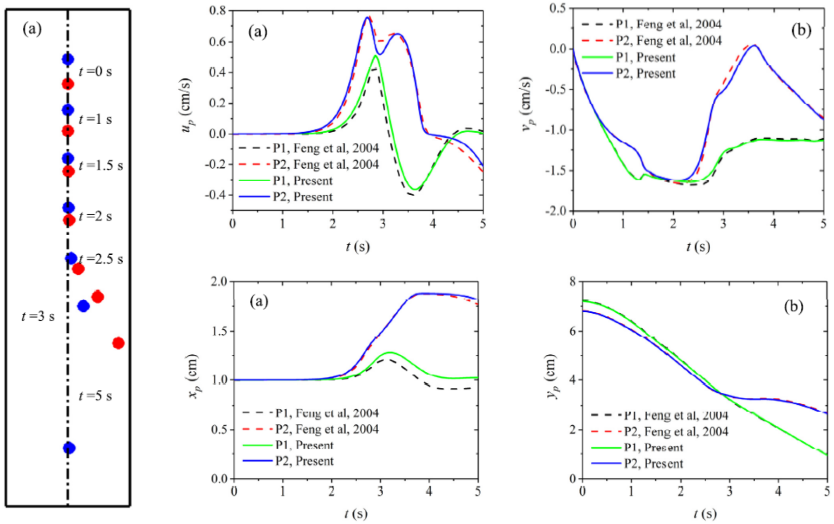


Conventional Present(improved)

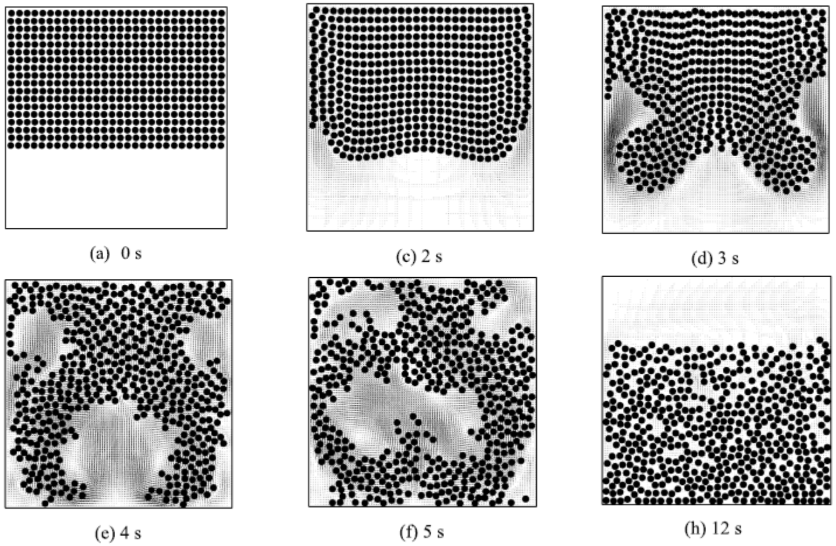
Flow past single cylinder (Re=40)

References	$Re=1$	$Re=40$		$Re=200$		
	C_D	C_D	Lw	C_D	C_L	St
Tritton [55]	10.92	1.62	–	–	–	–
Choi et al. [56]	–	1.52	2.25	1.36 ± 0.048	±0.64	0.191
Le et al. [57]	–	1.58	2.59	1.38 ± 0.040	±0.676	0.192
Park et al. [31]	12.00	1.54	–	1.35 ± 0.04	±0.65	0.192
Kang & Hassan [16]	–	1.597	2.525	–	–	–
Wu & Shu [20]	–	1.565	2.31	1.349	–	0.193
DF	11.266	1.556	2.42	1.39 ± 0.047	±0.720	0.198
IVC	11.278	1.551	2.40	1.360 ± 0.044	±0.670	0.192
RKPM	11.277	1.551	2.40	1.364 ± 0.042	±0.699	0.195
MDF ($NF=20$)	11.279	1.551	2.40	1.364 ± 0.042	±0.699	0.193
Present BTDF	11.277	1.551	2.40	1.364 ± 0.042	±0.699	0.195

Note: C_D and C_L for $Re=200$ are defined as $a \pm b$ with a mean value of a and a maximum deviation of b.



DKT of two particles sedimentation

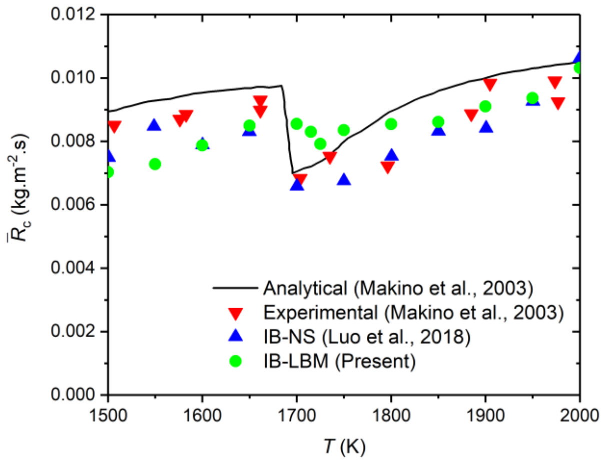


Rayleigh-Taylor instability of 504 particles

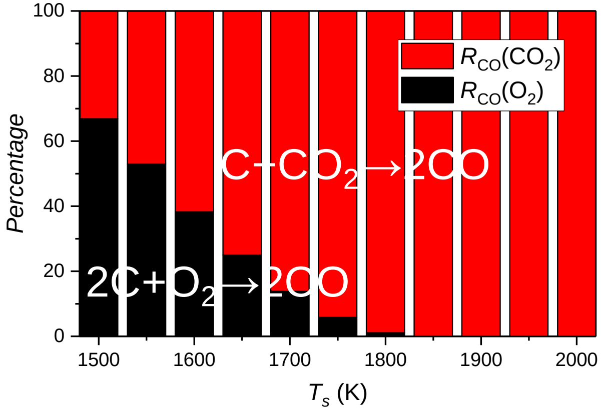
Non-slip boundary condition is satisfied.

3. Results and discussions

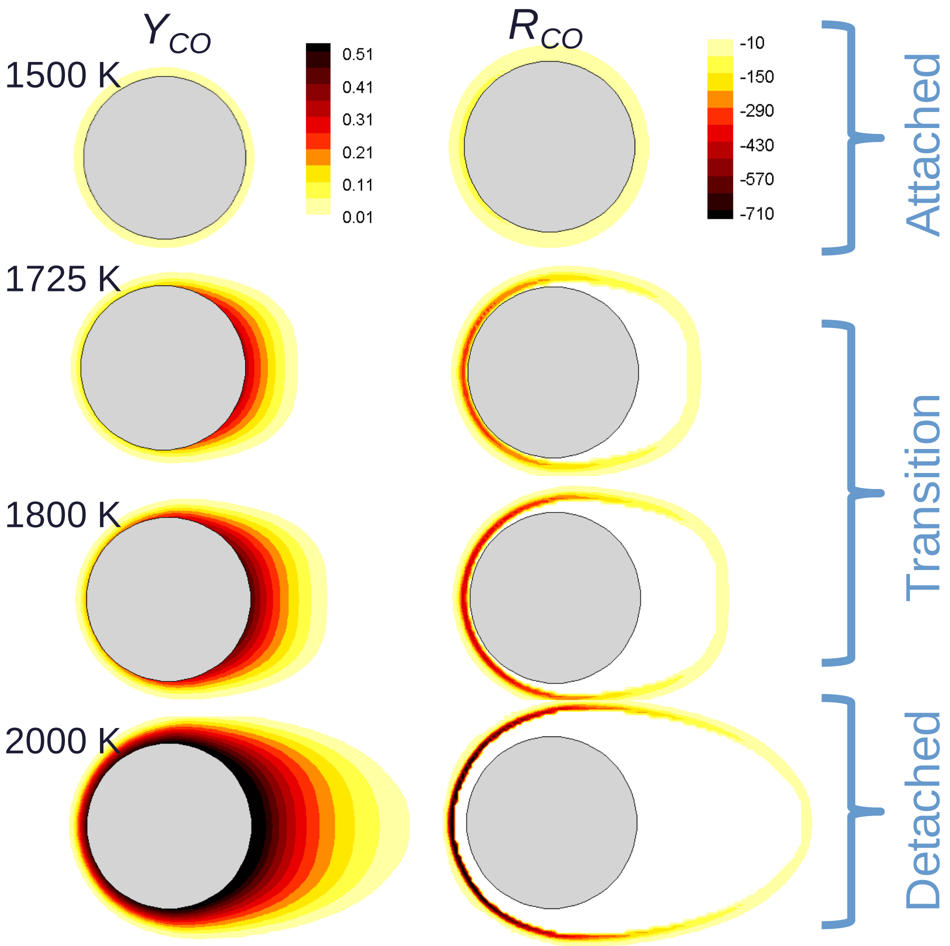
- Validation of char particle combustion



Carbon burning rate



Surface reactions evolution



CO mass fraction and CO flame around particle surface

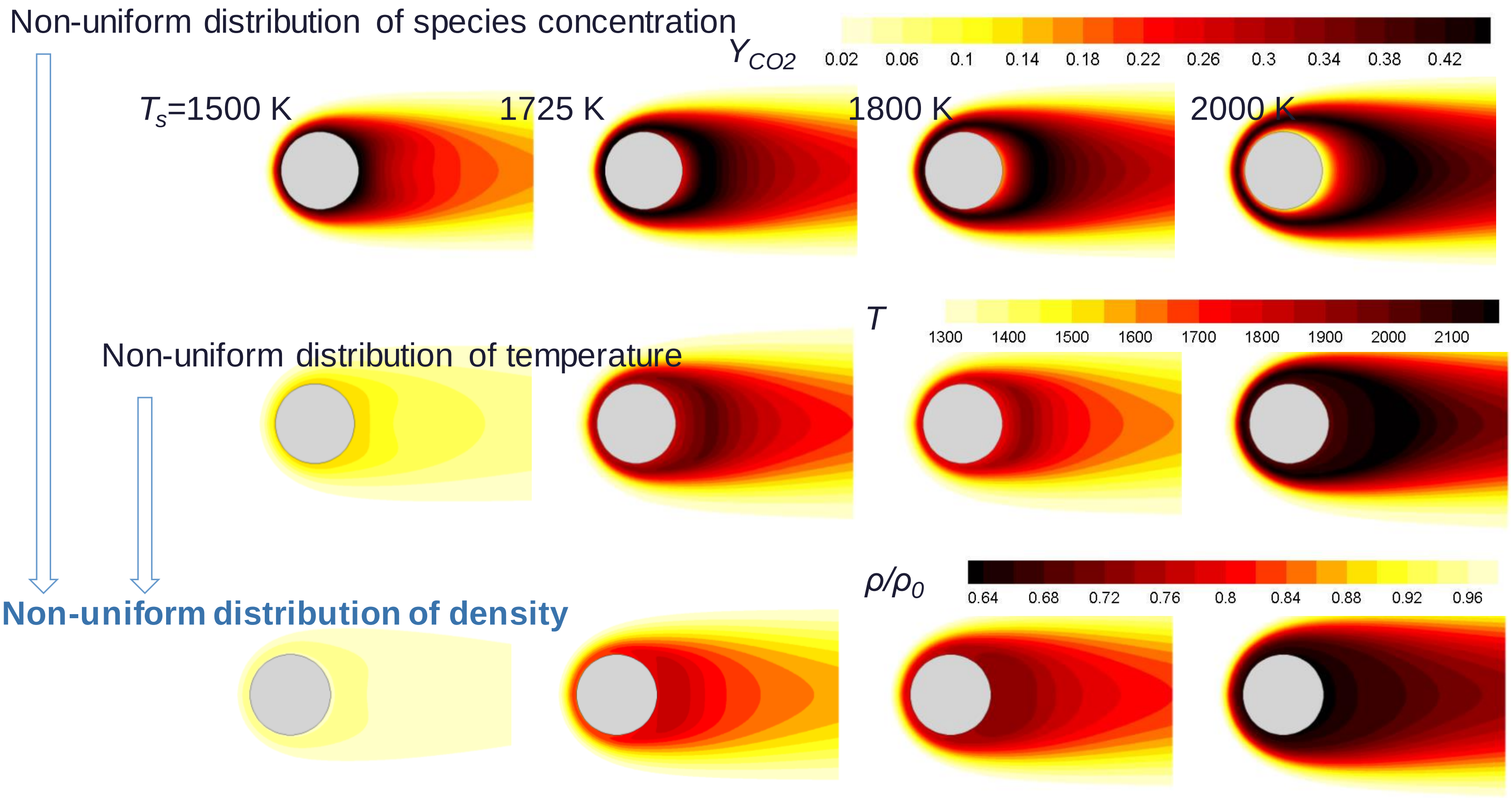
Simulation results agree well with previous experiments and simulations.

3. Results and discussions

- Variables around burning particle surface

➢ Large density fluctuations exist ($(\rho/\rho_0)_{max}$> 0.65) around particle surface due to non-uniform distribution of species concentration and temperature.

➢ High particle surface temperature T_s causes high density fluctuations ρ/ρ_0.



Non-uniform distribution of species concentration

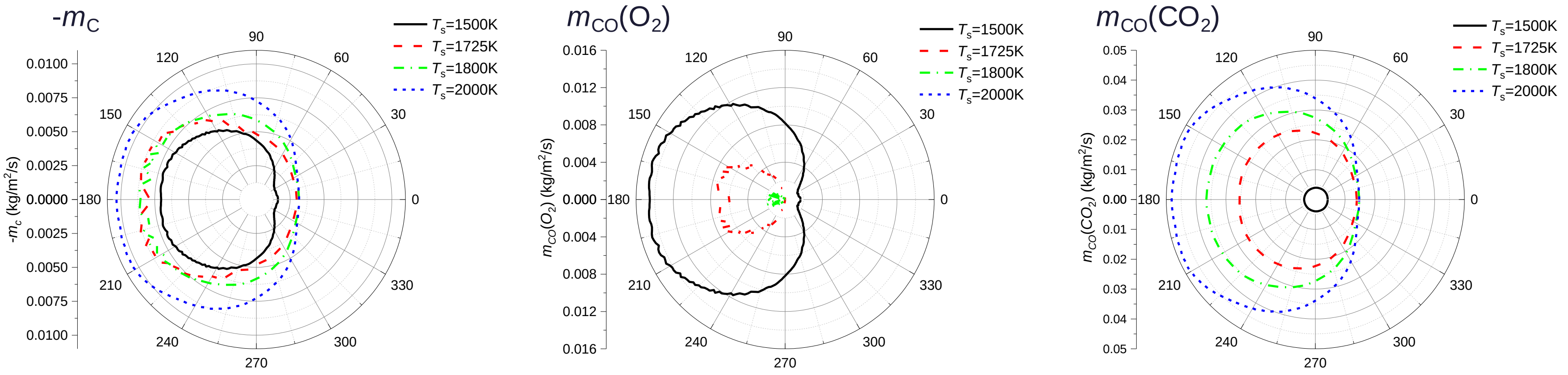
Non-uniform distribution of temperature

Non-uniform distribution of density

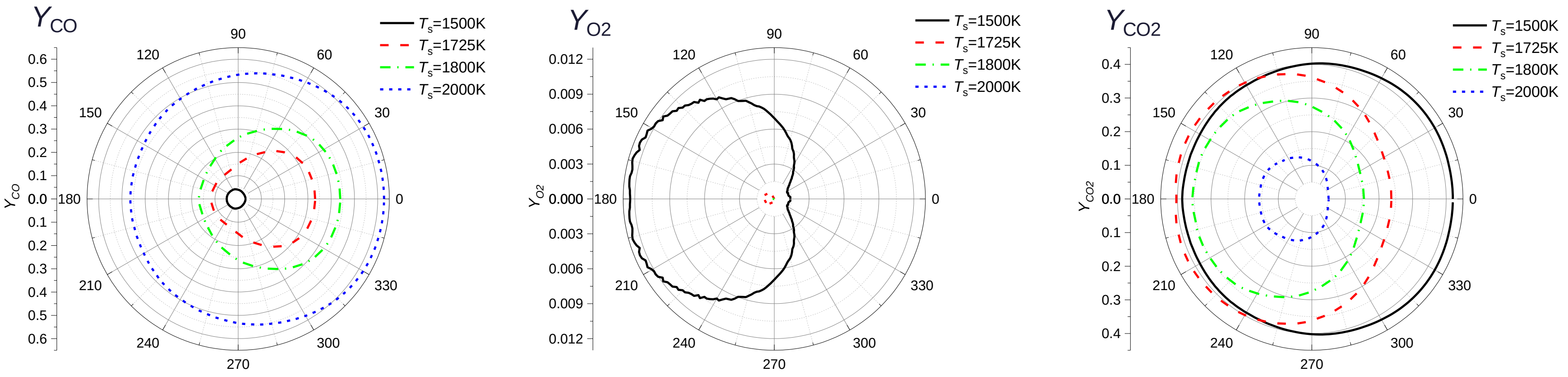
Large density gradient and fluctuations can be simulated.

3. Results and discussions

- Distributions of variables along particle surface



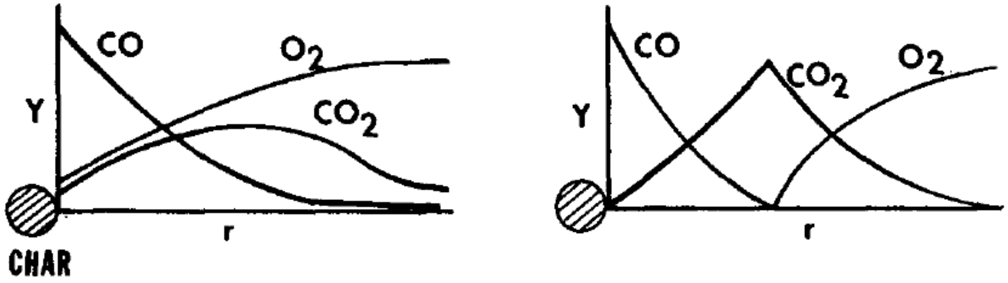
Distributions of reaction rates around particle surface



Distributions of mass fractions around particle surface

3. Results and discussions

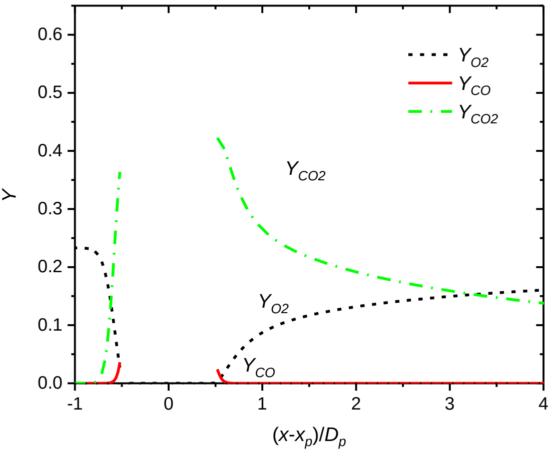
- Distributions of variables along particle centerline



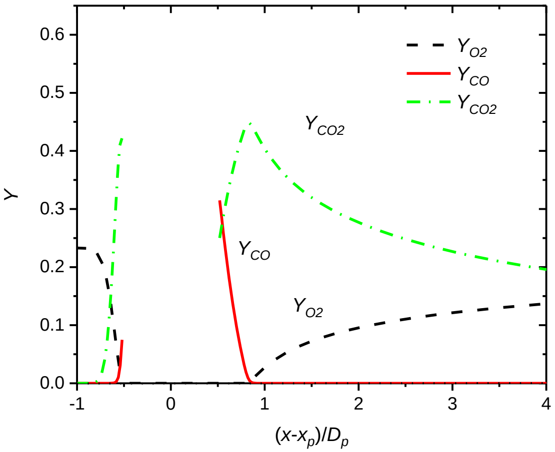
Single film model

Double film model

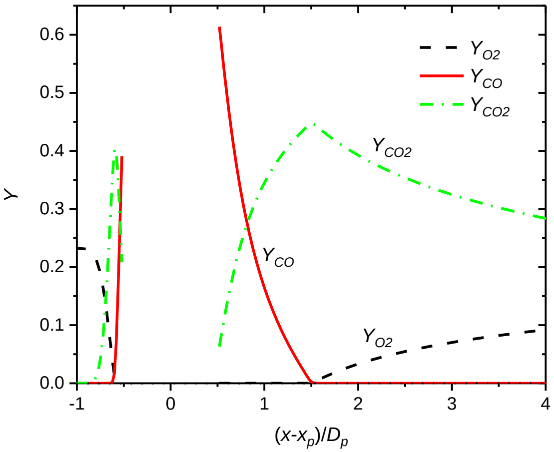
Conventional



T_S =1500K



T_S =1725K

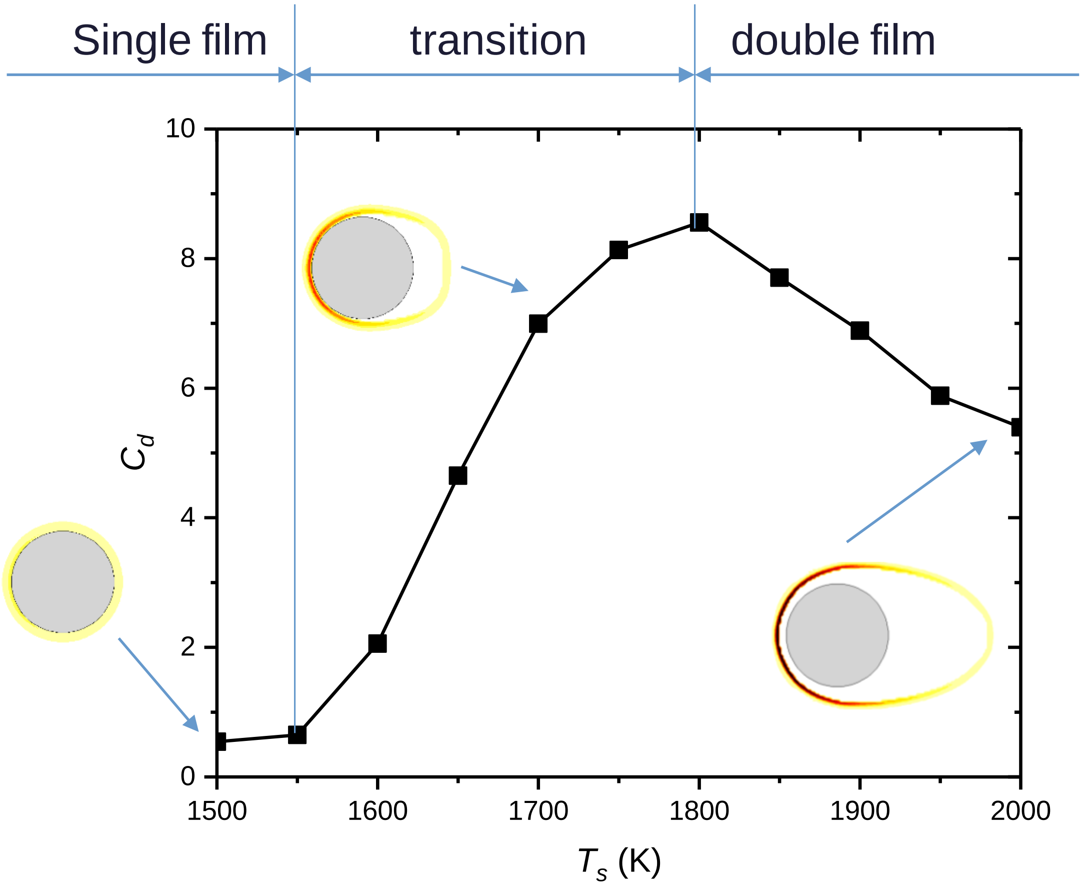


T_S =2000K

The actual distributions of species concentrations are much more complex than that obtained by conventional single film model (SFM) or double film model (DFM).

3. Results and discussions

- Drag force first increase and then decrease



4. Conclusions

- A new fully coupled IB-LBM method for gas-solid combustion has been presented.
- Three flame modes and large density fluctuations are simulated successfully.
- Char combustion is dominated by oxidation reaction to reduction reaction as particle temperature increases.
- Spatial distributions of species concentrations are much more complex than traditional single film model (SFM) and double film model (DFM).
- Drag force first increases and then decrease as the CO flame gradually detached.
- Future work: different inlet velocity, different inlet oxygen concentration, moving particle……

Thanks !