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Analysis of fluctuations in velocities, voidage and gas concentration in CFB conditions

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Background and motivation

- CFBs can be simulated reasonably well using CFD and fine mesh resolution
 - Computational requirements limit applicability
- Industrial scale applications require coarse meshes or time-averaged simulation
 - Closure models are needed for the time and length scales of the flow field that are not resolved
- Development of the closure models requires good understanding of the characteristics of the process



Background and motivation

- At VTT we have concentrated on the time-averaged approach for CFB combustion
- Filtered closure models for drag, solid pressure, volume fraction–pressure gradient correlation, inter-phase heat transfer
- A fluidization specific Reynolds stress turbulence model
- Promising results, however further development needed for e.g. chemistry
- Aim of the present study: gain more understanding of the fluctuation characteristics of chemical species in CFB conditions
- Method: simplified CFD simulation of combustion in a pseudo-2D riser





Time-scales, length-scales and diffusion coefficients

 Turbulent diffusion is a product of standard deviation of velocity fluctuation and Lagrangian length-scale

$$D_{T,i} = v_{\sigma,i} L_{L,i} \qquad v_{\sigma,i} = \sqrt{\overline{v'_i v'_i}} \qquad v_i = \overline{v_i} + v_i'$$

• The length-scale can be calculated from Lagrangian time-scale, defined with autocorrelation function $R_{L,i}$

$$L_{L,i} = v_{\sigma,i}\tau_{L,i} \qquad \tau_{L,i} = \int_0^\infty R_{L,i}(t)dt = \int_0^\infty \frac{v_i'(\tau)v_i'(\tau-t)}{v_{\sigma,i}^2}dt$$

- In this work the time-scales are calculated using Eulerian definition
- Eulerian and Lagrangian time-scales are not the same! Different ratios have been reported in even in single phase flows

$$v_{\sigma}\tau_L/\bar{u}\tau_E = 0.15 \dots 2$$
 $\tau_L/\tau_E = 1.7 \dots 4$





Numerical case setup

- Simulation carried out with OpenFOAM®, twoPhaseEulerFoam
- Included species O₂, CO, CO₂, N₂
- Single step combustion reaction

$$\operatorname{CO}(g) + \frac{1}{2}\operatorname{O}_2(g) \to \operatorname{CO}_2(g)$$

- CO released directly proportional to local solid volume fraction, global $\lambda = 1.0$
- Reaction rate limited by reaction kinetics and EDM turbulent rate (k, ϵ from Smagorinsky LES)

$$R_{kin} = A_r e^{-\frac{E}{RT}} [CO] [O_2]^{1/2} [H_2 O]^{1/2} M_{CO}$$
$$R_{turb} = \alpha \rho_g \frac{\epsilon}{k} A \min\left(\frac{Y_{CO}}{M_{CO}}, 2\frac{Y_{O_2}}{M_{O2}}\right) M_{CO}$$





Numerical case setup cont.

Physical parameters	
Dimensions	14x3x0.05 m
Fluidization velocity	2.5 m/s
Particle diameter	200 µm
Particle density	2500 kg/m3
Temperature	1170 K
Mesh resolution	12.5 mm
Cell count	800 k
Time step	<0.25 ms
Simulated time	80 s

Numerical Models	
Granular viscosity	Syamlal
Granular conductivity	Syamlal
Granular pressure	Lun
Frictional stress	Schaeffer
Radial Distribution	SinclairJackson
Drag	Gidaspow



Results: transient and time-averaged fields

- O₂ concentration is high at the bottom, small near walls
- CO₂ and O₂ have opposite behavior

- Concentration of CO is mostly small, high near walls
- Length scales of O₂ and CO₂ similar to velocity field, CO similar to volume fraction field





Eulerian time scales

- Anisotropic and large locational dependence
- Solid phase time scales are longer than gas phase
- Fluctuation time scales of volume fraction are relatively uniform, shorter than those of velocity



- O2 and CO2 time scales roughly equal to velocity time scales
- CO has large spatial variance in the time scales; small time scales at the bottom, large near walls





Diffusion coefficients

- Horizontal diffusion is large at the very bottom, overall vertical diffusion is larger
- Vertical diffusion increases with height, horizontal diffusion is largest at the center
- Gas phase diffusion larger than solid phase





Time averaged reaction rates

- In most parts of the riser the turbulent reaction rate has limited the reactions
- Based on the averaged concentrations, CO has usually limited the reaction rate
- Overall reactions have been fast compared to the source



The ratio of the average reaction rate to the local scale turbulent reaction rate

O₂ limited areas



Examples of fluctuation patterns

 At the bottom CO concentration closely follows solid volume fraction

 Higher up the CO no longer follows solid volume fraction, O₂ and CO are linked

 Near to the wall O₂ only occasionally spikes





Results: example energy spectrum

- Largest energy at small frequencies, no clear peaks
- Typically gas velocity has larger fluctuations than solid, vertical fluctuations larger than horizontal
- Depend on position, eg. near walls horizontal fluctuations are small
- Species fluctuation spectrums are similar





Reaction rate in time-averaged simulation

- How to calculate reaction rate from time-averaged variables?
- Simplest approach Eddy-Dissipation model

$$R_{eff} = \bar{\alpha} \, \overline{\rho_g} \frac{1}{\tau_{\rm R}} \, A \, \min\left(\frac{\overline{Y_{co}}}{M_{co}}, 2 \frac{\overline{Y_{O_2}}}{M_{O2}}\right) M_{CO}$$

- Ideally $R_{eff} = \overline{R}$
- Question 1: what τ_R should we use?
- Question 2: can τ_R be obtained easily from the flow time scales?

$$\tau_R = C_{R\alpha} \tau_\alpha \qquad \qquad \tau_R = C_{Ru} \max[\tau_{E,x}(u_g), \tau_{E,y}(u_g)]$$



Time scales for EDM-type reaction rate

- Required reaction time scale is not uniform
- Time scale does not directly resemble flow time scales -> constant correction does not work
- At the middle, the volume fraction time scales work quite well, near walls velocity scales are slightly better





Future work

- More simulations with varying conditions are needed
 - Different stoichiometric ratios, secondary air inlets
- Sensitivity studies for reaction rate
 - How the situation changes if reactions are slower or faster?
 - Effect of the turbulent reaction rate assumptions

For time averaged reaction rate model:

- Validation of the transient reaction rates in small scale/pilot scale
- Include varying temperature and H₂O concentration, CO release from fuel particles



Summary

- Simplified CFD simulation of combustion in a CFB was performed
- Fluctuation time scales were determined for velocity, voidage and gas species concentrations
- The time scales strongly depend on the location in the riser and on flow conditions
- Applicability of Eddy-Dissipation type reaction model for timeaveraged simulation was investigated

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