Simulation of soot size distribution in an ethylene counterflow flame

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Introduction

Soot, an aggregate of carbonaceous particles produced during the rich combustion of fossil fuels, is an undesirable pollutant and health hazard. Soot evolution involves various dynamic processes:

nucleation soot formation from polycyclic aromatic hydrocarbons (PAHs)

condensation PAHs condensing on soot particle surface

surface processes hydrogen-abstraction-C_2H_2-addition, oxidation

coagulation two soot particles coagulating to form a bigger particle

This simulation work investigates soot size distribution and morphology in an ethylene counterflow flame, using i). Chemkin with a method of moments to deal with the coupling between vapor consumption and soot formation; ii). Monte Carlo simulation of soot dynamics.

Methodology

Soot dynamics

The soot particle size distribution function n satisfies a population balance equation

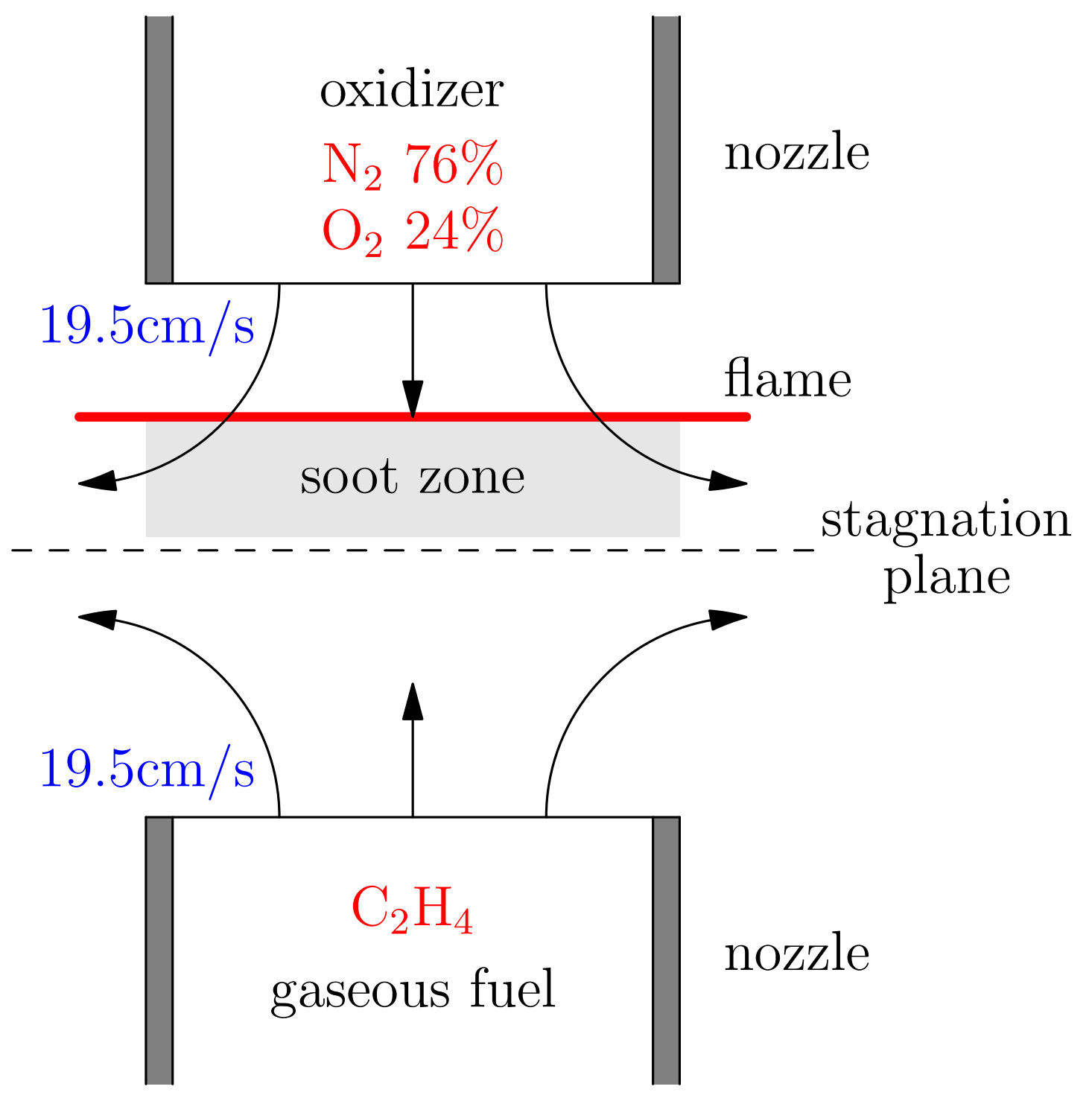
$$\frac{\partial n}{\partial t} + \nabla \cdot n\vec{u} = \left[\frac{\partial n}{\partial t}\right]_{\mathrm{nuc}} + \left[\frac{\partial n}{\partial t}\right]_{\mathrm{cond}} + \left[\frac{\partial n}{\partial t}\right]_{\mathrm{surf}} + \left[\frac{\partial n}{\partial t}\right]_{\mathrm{coag}}. \qquad (1)$$

In the counterflow configuration studied here, u is the gas axial velocity. The soot dynamics can be described by the following collision model

$$R = C_E \times \beta_{a,b} \times C_a \times C_b, \qquad (2)$$

where a and b denote the two collision parts, and C_a and C_b are their concentration. C_E is the collision efficiency, and $\beta_{a,b}$ is a function that measures the collision frequency. The equation describes the rate for nucleation (PAH + PAH), condensation (PAH + soot), surface reaction (oxidizer + soot), and coagulation (soot + soot). Here, the KAUST mechanism [1] is used, which includes eight PAHs, from pyrene ($C_{16}H_{10}$) to coronene ($C_{24}H_{12}$).

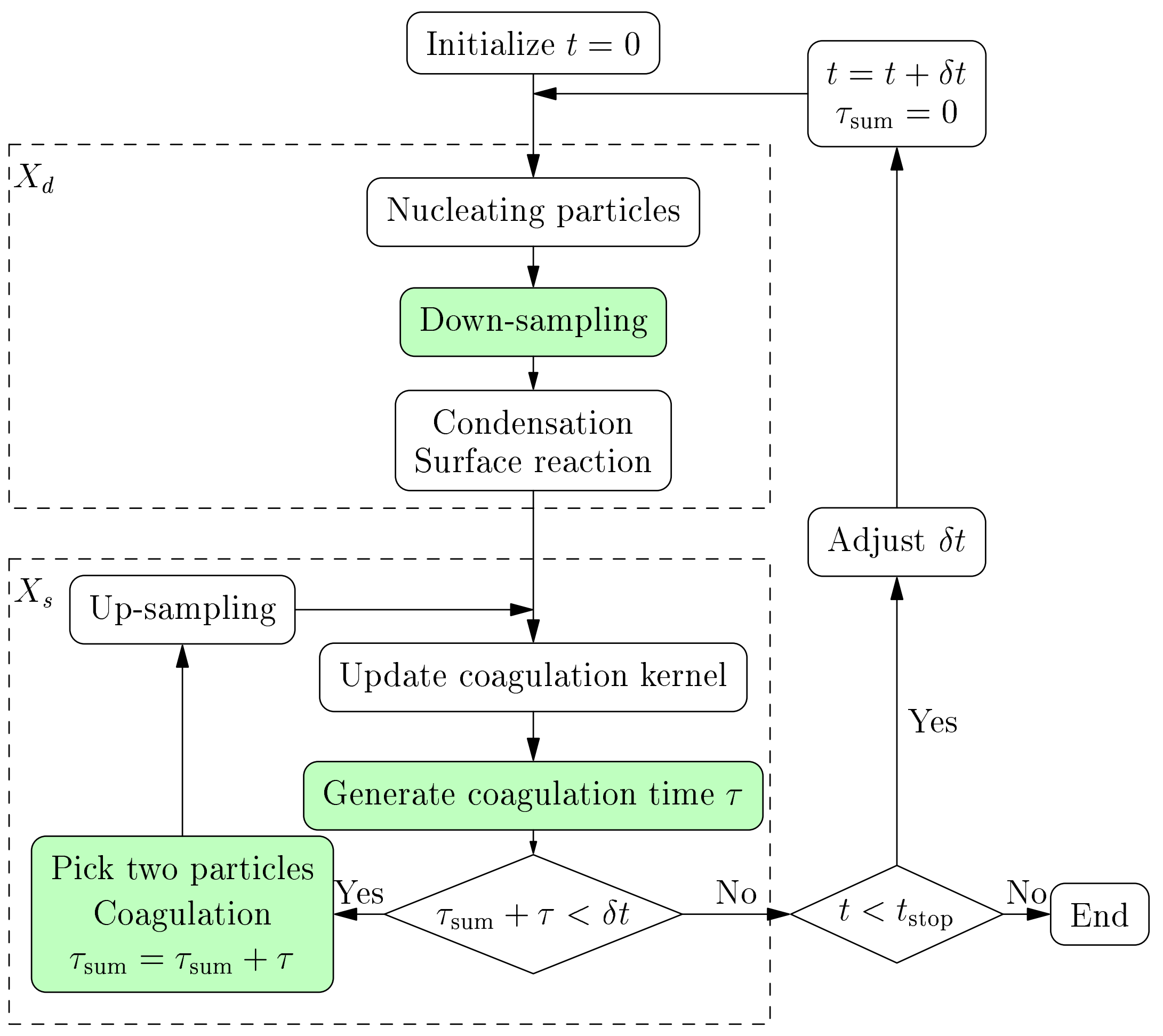
Counter flow configuration



The flame is located on the oxidizer side of the counterflow. Soot particles formed on the fuel side of the flame are transported away from the flame and towards the stagnation plane, following the streamlines closely [2].

Monte Carlo scheme

The Monte Carlo scheme uses operator splitting technique to combine stochastic simulation of coagulation and deterministic integration for nucleation, condensation and surface growth.



References

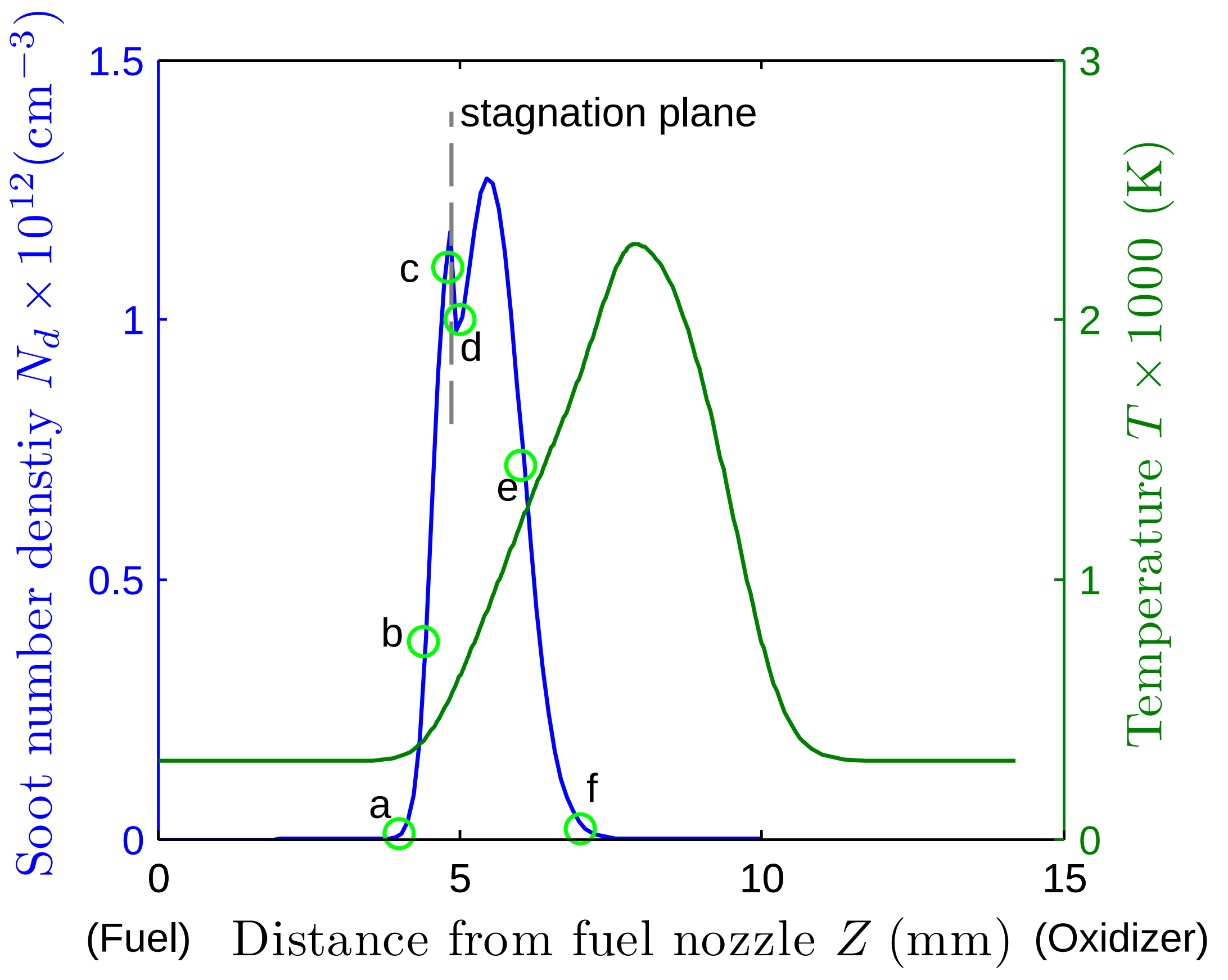
[1] A. Raj, I.D. Prada, A.A. Amer, and S.H. Chung, *Combust. Flame*, 159:500–515, (2012).

[2] B.C. Choi, S.K. Choi, S.H. Chung,J.S. Kim, and J.H. Choi, *Int. J. Automot. Technol.*, 12:183–191 (2011).

Profiles

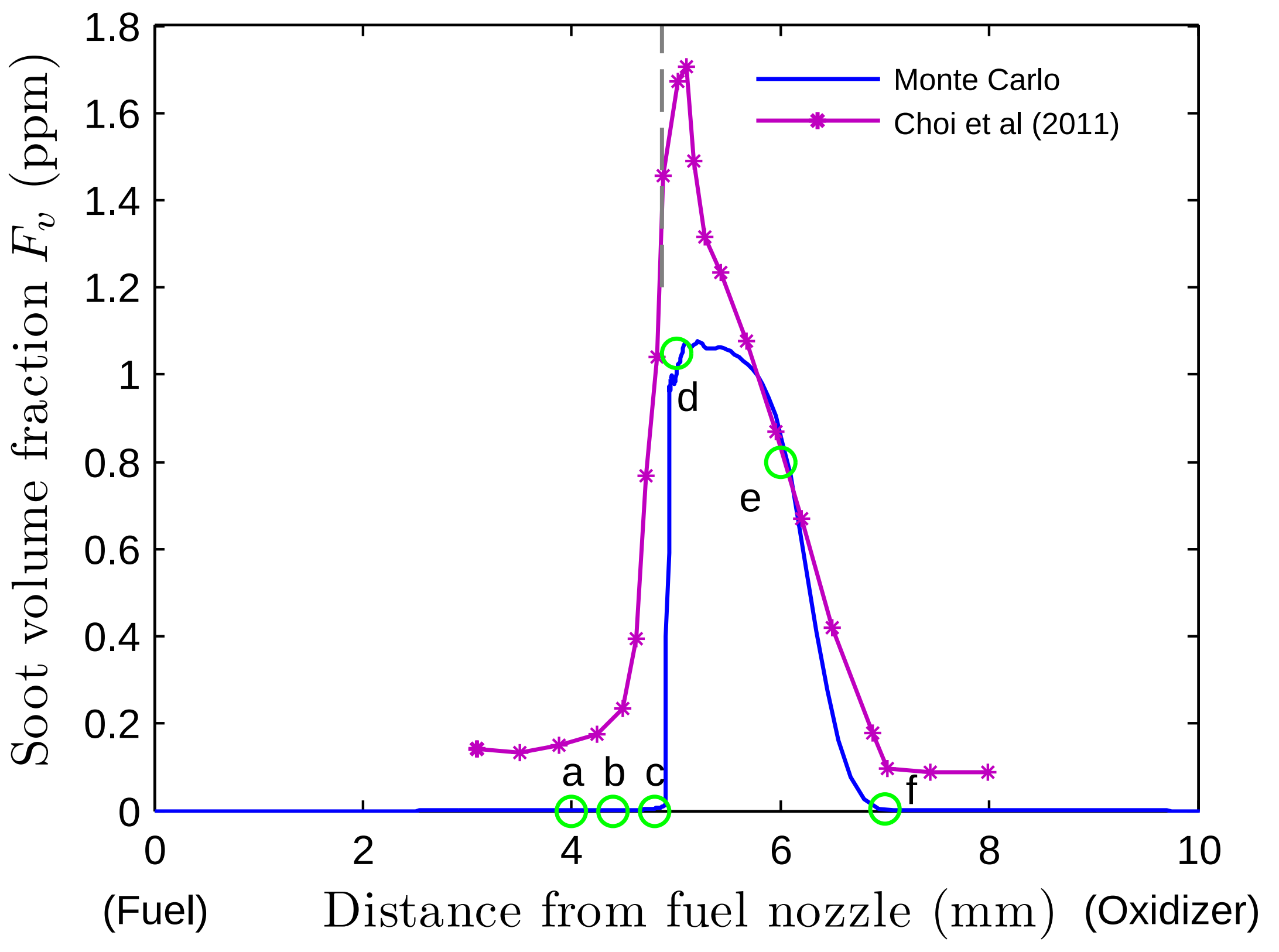
Soot number density

Soot particles are formed away from the flame (peak temperature), and the number density approaches the maximum near the stagnation plane. A dip of the number density at the stagnation plane is due to strong coagulation and diminished nucleation.



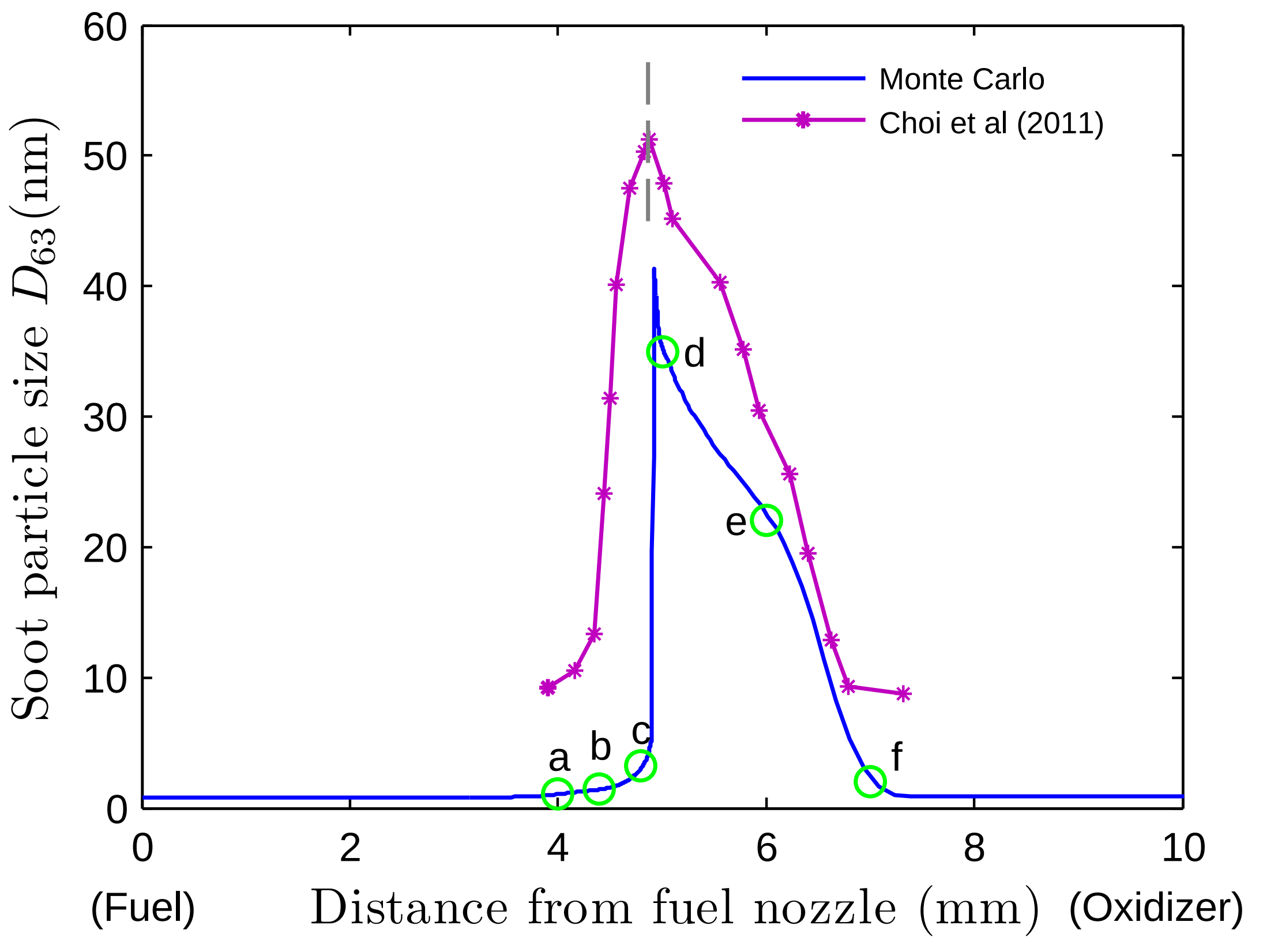
Soot volume fraction

Volume fraction increases towards the stagnation plane from the oxidizer side, and decreases sharply away from the plane on the fuel side.



Soot particle size

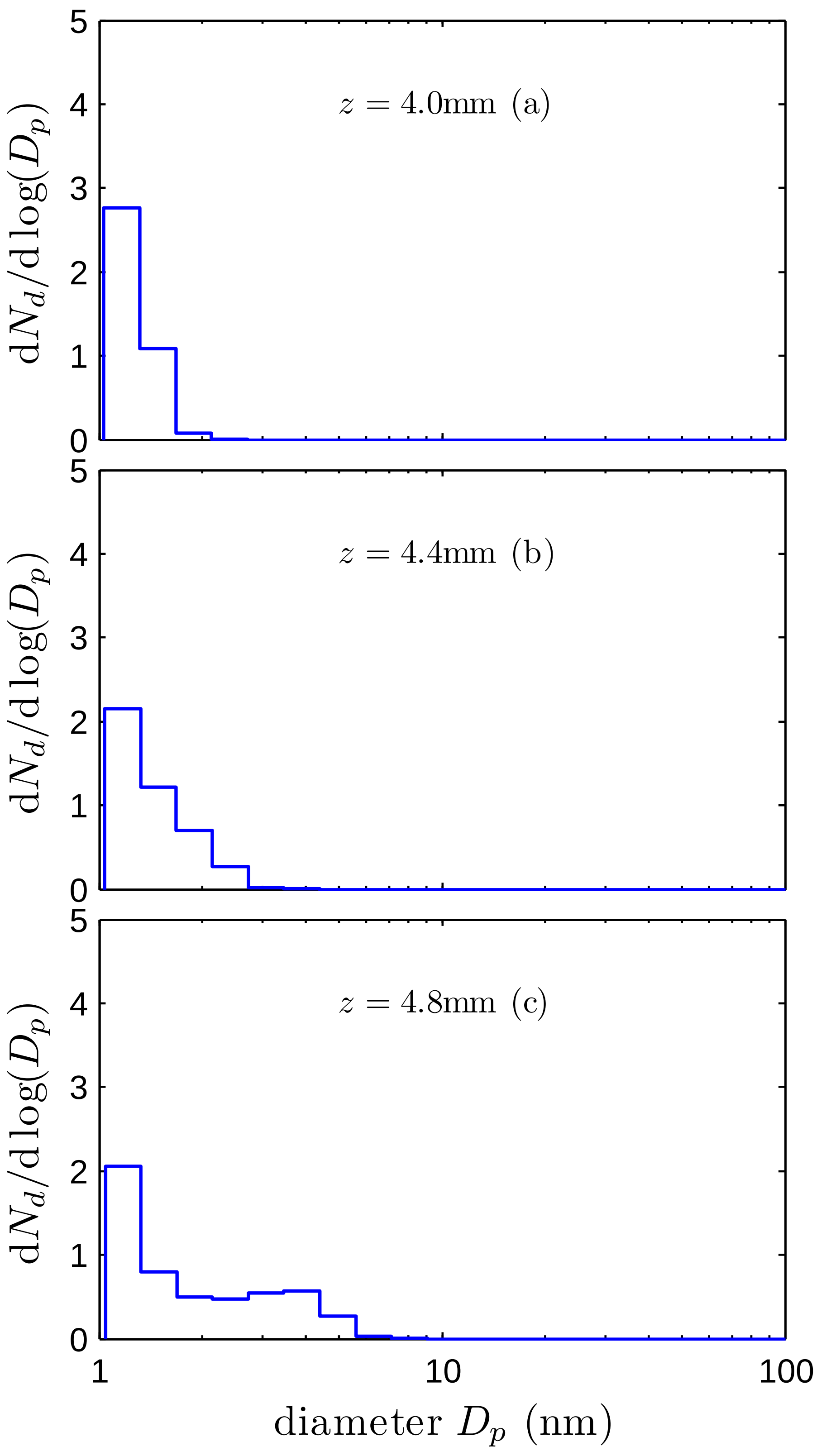
The particle size D_{63} is defined as $D_{63} = (M_6/M_3)^{1/3}$ (where M_6 and M_3 are the sixth and third order moments with respect to the diameter), which is the mass mean diameter. Near the stagnation plane, particles grow very fast mainly due to coagulation for long residence time.



Soot particles size distribution (PSD)

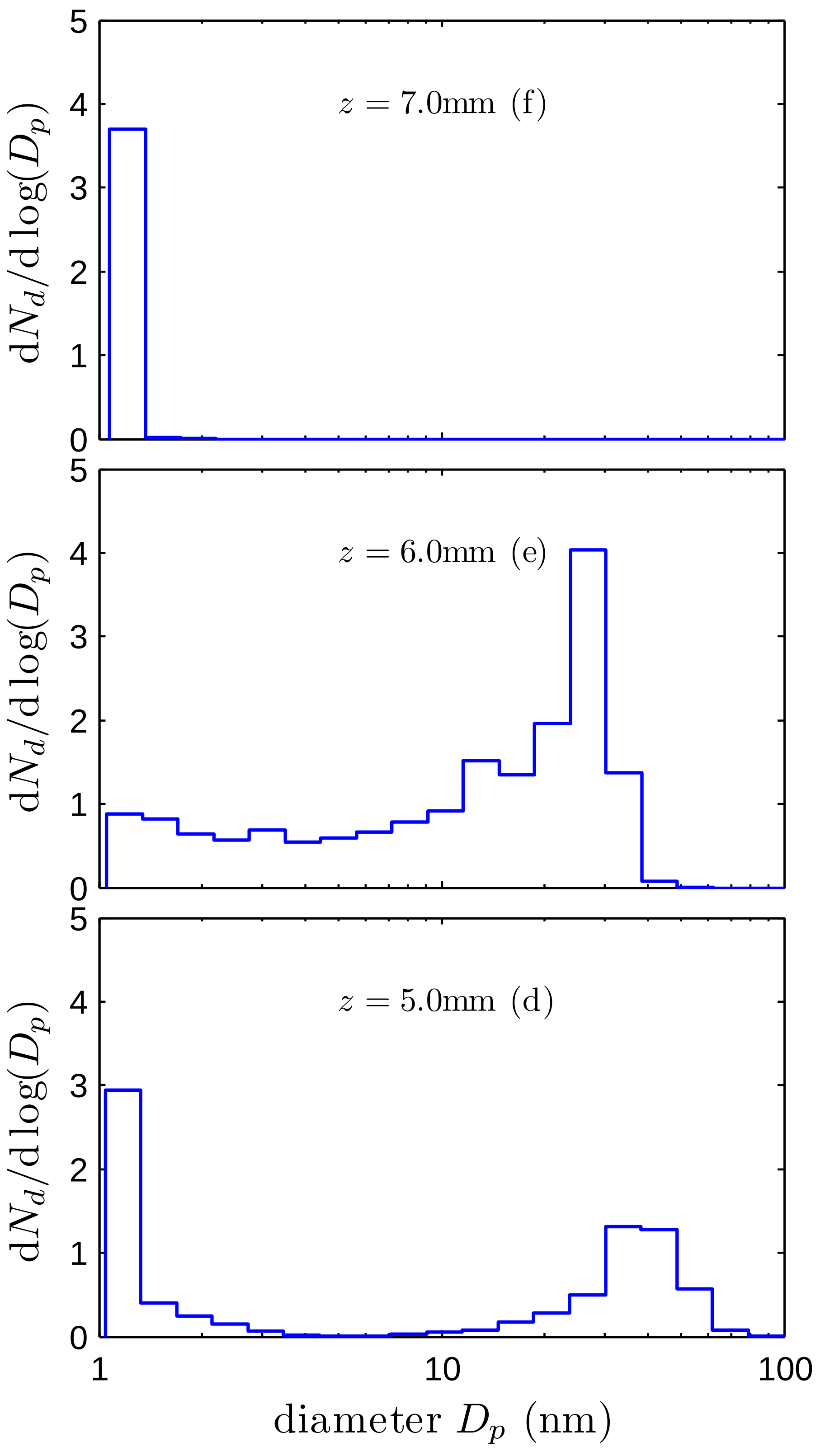
Soot particles are assumed to be spherical, with diameter D_p.

On the fuel side



- PSD has a peak at nucleated particles size, and has longer tail towards the stagnation plane.
- Nucleation is active (see the N_d profile).
- Particles are small due to weak growth.

On the oxidizer side



- All soot dynamics are active.
- PSD evolves from a delta peak (due to nucleation), to a plateau (due to condensation and surface reaction), and to a bimodal distribution (due to coagulation).
- Particles size growth is mainly due to coagulation.