Lattice Boltzmann Simulation of Heterogeneous Reactions for Soot Filter Regeneration

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Highlights

- Lattice Boltzmann simulation of heterogeneous combustion with conjugate heat transfer
- Analysis of the combustion regime
- Morphology evolution of realistic soot geometry from FIB-SEM imaging

1. Introduction

Automotive soot filtering is of great interest in the prospect of harsher political regulations and higher public conscience on health effects and effects on the climate. State of the art soot filters are cermaic wall flow filters, resulting in the formation of a soot cake. The filtration in this soot cake then provides the main filtration performance, albeit resulting in an increasing filter backpressure, making regeneration imperative. To study the regeneration process and the influence of the soot morphology onto the reaction rate, a Lattice Boltzmann (LB) model is set-up and simulations with realistic soot geometries, obtained from FIB-SEM images, are performed.

2. Methods

For the simulation of soot combustion, a model, which incorporates multi component flow in porous media, the temperature field, fluid-solid interactions and heterogeneous reactions, is necessary. Here, the Lattice Boltzmann method is used for this purpose. This method is based on modelling the statistical distribution of the movement of molecules on the mesoscopic scale, following a so-called bottom-up approach. The basic LB transport equation utilizing the BGK [1] approximation for the collision term is shown in equation (1, consisting of the streaming step on the left and the collision step on the right. Furthermore, external forces are represented here by the Guo forcing scheme [2]. With the transport equation being explicit in time and fully local, calculations can be performed in a parallelized manner.

$$f(x + c_i\Delta t, t + \Delta t) - f(x,t) = -\frac{1}{\tau}[f(x,t) - f^{eq}(x,t)] + \Delta t\left(1 - \frac{1}{2\tau}\right)\mathrm{F} \qquad (1)$$

This equation, when upscaled using the Chapman-Enskog expansion, resembles the Navier-Stokes equation for fluid flow. For the temperature field and component fields, similar transport equations can be formulated, making it possible to simulate soot combustion with a full LB model. As a note, the basic transport equations are similar to the ones presented in [3], with the distinction that the conjugate heat transfer algorithm presented in [4] is used.

3. Results and discussion

In a first step, the combustion regime was to be examined. For this purpose, a 2D simulation domain, consisting of regularly ordered round soot particles, was created. In this domain, a velocity profile as well as fix values for the temperature and component fractions were imposed at the inlet, and zero gradient boundary conditions, enforcing a fully developed flow, were imposed on the outlet. Then, the inlet mass fraction of the educt, oxygen, as well as the Péclet number was varied. The results are displayed in *Figure 1*, where it can be seen that the propagation velocity of the combustion front is nearly proportional to the inlet mass fraction of oxygen and describes an exponential dependency from the Péclet number. This is expected since for $Pe<0.1$, the diffusive mass transfer is dominating, resulting in a diminishing effect of Pe on the overall mass transport. For $Pe>0.1$, the advective mass transport is dominating, resulting in higher propagation velocities for the mass transfer limited combustion regime.

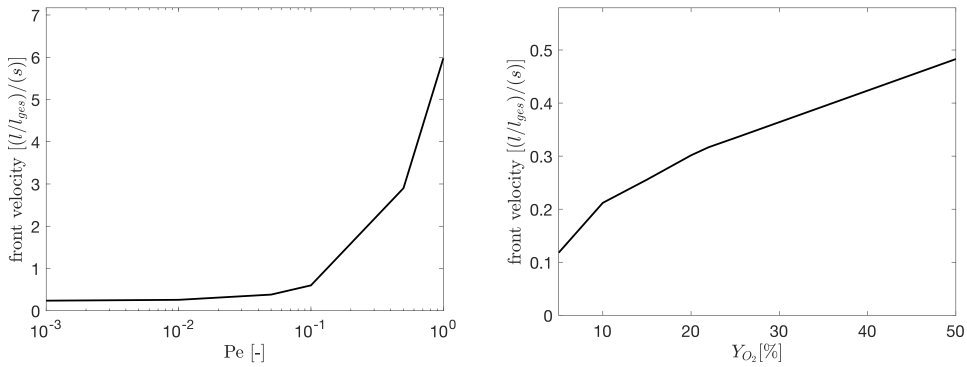

Figure 1. Propagation velocity of the combustion front for different Péclet numbers (left) and inlet mass fractions of oxygen (right).

Subsequently, a realistic soot geometry is used for the combustion simulations, and the evolution of the morphology is studied. The change of the morphology and specific surface are shown in *Figure 2*. It can be seen that a combustion front propagates through the domain, resulting in the soot not being consumed homogeneously, but rather being consumed progressively in streamwise direction. This results in a near constant specific reactive surface.

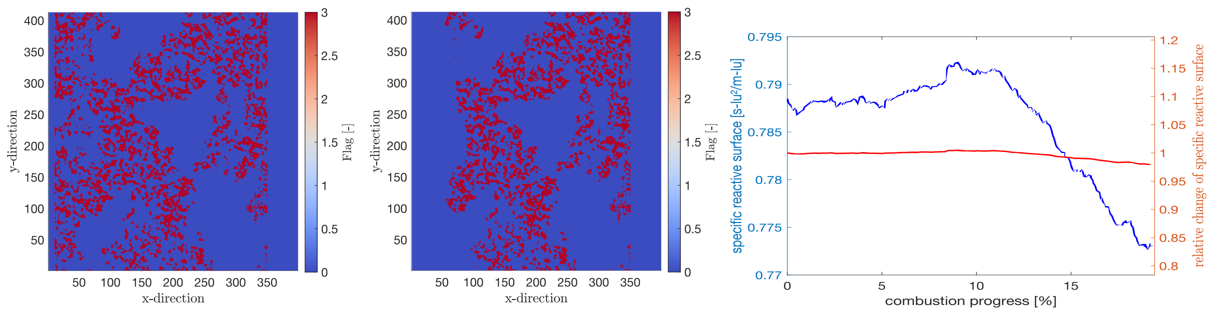

Figure 2. Temporal evolution of the soot geometry. Initial geometry (left) and geometry at 40 µs (right). One lattice spacing is equivalent to 10 nm.

4. Conclusions

A code to study the combustion of porous soot structures using LBM was created and a parametric study was conducted to analyze the combustion behavior.

References

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Keywords

Heterogeneous Reaction; Porous Media; Lattice Boltzmann Method