ON MODELLING AND SIMULATION OF AUTO-IGNITION IN PARTICLE-LADEN BIOMASS FLOWS

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Abstract. This study focuses on the safety-critical problem of auto-ignition in particle-laden flows, where biomass particles enter a computational domain, form deposition layers ("cake"), and are susceptible to ignition due to thermal and chemical interactions. Such scenarios are particularly relevant in storage silos, biomass processing plants, and industrial systems, where ignition can lead to deflagration, causing safety hazards and operational disruptions. In previous works we have used the finite volume techniques implemented in the Octave/Matlab environment and have simulated the temporal evolution of solute distribution and solvent velocity in two and three dimensions. The modified equations for a system with moving particles in Lagrangian coordinates have been solved. As a result, we have observed the behaviour of different portions of particles and the appearance of certain layer-type patterns – something of a wide interest in different applications. The modular framework we have created can accommodate custom laws, offering versatility across industrial contexts. To address the current issue, we discuss the applications of particle motion equations with combustion models derived from the Navier-Stokes framework, accounting for heat transfer, species transport, and chemical reactions. The ignition mechanism is characterized by coupling the thermal energy equation with pyrolysis kinetics to simulate volatile release and heat feedback in the system. Critical parameters, such as layer thickness, oxygen concentration, heating rates, and ambient conditions, can be systematically varied to identify ignition thresholds. These findings have a potential of a framework for engineers to design safer biomass storage and processing environments by understanding and controlling the conditions that lead to ignition. This work serves as a foundation for further research on combustion-driven safety in industrial particle-laden systems.

Keywords: particle-laden flows, Navier-Stokes, combustion modelling, Lagrangian particle tracking, biomass deposition.

Introduction

Biomass fuels have become widely used in power generation and industrial processes as a renewable energy source. However, storing and handling large quantities of biomass introduces serious safety concerns due to the risk of spontaneous combustion. Self-heating of biomass during storage can lead to auto-ignition without any external spark, causing fires or even dust explosions [1]. Several biomass storage facilities have suffered such incidents in recent decades, therefore there is a need for better predictive understanding and prevention mechanisms.

Auto-ignition in biomass is driven by a combination of physical, biological, and chemical processes that gradually generate heat within the bulk material. Moisture adsorption and condensation can release latent heat, microbial metabolism in moist organic matter produces heat, and slow oxidative reactions (often at the particle surfaces) further contribute to exothermic energy. Because raw biomass typically has low thermal conductivity, the heat generated by these processes tends to be trapped inside densely packed piles or silos instead of dissipating to the environment. This self-heating effect can accelerate with rising temperature, creating a positive feedback loop that may eventually lead to thermal runaway and ignition.

Numerous studies have investigated this self-heating phenomenon through experiments and modelling. Small-scale trials (e.g. in insulated containers or basket tests) have been used to measure temperature rise and ignition delay in various biomass fuels, providing data to validate numerical models [2]. On the theoretical side, researchers have developed models to predict when and where spontaneous ignition will occur. Early analytical approaches have found basic ignition criteria but required simplifying assumptions for geometry and reaction kinetics. With advances in computational power, more detailed simulations have become possible [3; 4]. Fluid flow simulations, based on the Navier–Stokes equations, have been introduced to describe the convective transport of heat and oxidant within biomass deposits. Accounting for airflow is important because buoyancy-driven ventilation (the "chimney effect") can significantly change the temperature distributions inside a porous biomass pile. For example, [5] implemented a three-dimensional two-phase CFD model for wood pellets that included gas flow, heat transfer, and oxygen consumption, and they showed that including convective effects improved agreement with laboratory self-heating experiments. In [6], likewise, a mathematical model

has been developed for large open wood chip piles, incorporating heat generation from oxidation, microbial activity, and moisture interactions, and reported good agreement between their simulated temperature profiles and field measurements in industrial-scale piles. In [7] the CFD framework has been proposed that deals with physical, chemical, and microbial processes to predict the auto-ignition zones in biomass storage systems. These studies show that a simulation approach must resolve both the reactive heat source in the biomass and the transport processes (heat and mass transfer) that tells us whether the heat accumulates or dissipates. Understanding the detailed ignition mechanisms helps inform better ventilation strategies and early-warning monitoring to prevent fires [8].

Despite these advances, modeling auto-ignition in particle-laden biomass flows remains challenging. Biomass storage beds consist of discrete particles (e.g. pellets, chips) with complex pore networks for air flow, making the heat and mass transfer highly heterogeneous. Simplified models that treat the pile as a continuum, may not capture local hot spots or the detailed connection between particles and the surrounding gas. This has motivated the use of Navier–Stokes-based simulations that track the coupled behavior of the fluid and solid phases with high resolution. By utilizing a Eulerian–Lagrangian framework, it becomes possible to follow each particle's trajectory and thermal state within a flowing system, while the Navier–Stokes equations describe the carrier gas flow and convective heat exchange. This level of detail is especially beneficial for capturing ignition phenomena, since auto-ignition often starts in localized regions around individual hot particles or poor ventilation zones.

In this paper, we continue the work [9; 10] and present a simulation approach for auto-ignition in a particle-laden biomass flow. The proposed model couples the Navier–Stokes equations for the gas phase with heat conduction and reactive source terms for the biomass particles, allowing us to simulate the growth of hot spots and the onset of ignition in realistic flow configurations. By performing three-dimensional simulations under various storage conditions, we can identify the critical combinations of parameters that lead to self-ignition. The outcomes of this study are directly applicable to engineering practice – for instance, in designing safer pellet silos, storage piles, and conveying systems.

Materials and methods

We propose a system of partial differential equations consisting of fluid dynamics equations (1)-(2), describing the flow:

$$\frac{\partial v}{\partial t} + \nabla \cdot (v \otimes v) = -\nabla p + \frac{1}{Re} \triangle v + f, \tag{1}$$

$$\nabla \cdot v = 0 \tag{2}$$

and we additionally apply suitable boundary conditions for velocity and pressure, including homogeneous Neumann conditions for pressure at the rigid walls, either pressure or velocity conditions at the inflow, and Dirichlet pressure at the outlet.

Regarding the particle tracking in the flow, their dynamics are described by their COG dynamics, influenced by hydrodynamic forces and gravity forces:

$$m_i \ddot{x_i} = F_H + \frac{\rho_s - \rho_f}{\rho_s} m_i g. \tag{3}$$

Here dots over variables denote the time derivative, ρ_s and ρ_f denote density of the biomass particles and solvent respectively and the hydrodynamic force acting on the i-th particle is

$$F_H = C_D(v(x_i, t) - \dot{x_i}) \tag{4}$$

and C_D is the total drag coefficient. For computations in the present article, we use the Stokes drag for a sphere with a radius a:

$$C_D = 6\pi\mu a. \tag{5}$$

The force the particles exert on the fluid is modelled by the 3d Gauss kernel:

$$W(x) = (2\pi\sigma^2)^{-\frac{3}{2}} exp(-x^2/2\sigma^2), \tag{6}$$

where σ – related to the particle radius a.

By the third Newton's law, the back-coupling force exerted by the particles on the fluid is

$$f(x,t) = -\sum_i F_H \cdot W\big(x - x_i(t)\big). \quad (7)$$

In the presence of buoyancy or sedimentation of the particles we need to consider particle collisions with walls. We treat them as inelastic collisions: normal velocity component to the wall is set to zero in case of contact (particle sticks to the wall).

The temperature evolution in the system is governed by the energy equation, incorporating convective transport, thermal diffusion, and reaction-generated heat:

$$\rho c_p \frac{DT}{Dt} = \nabla \cdot (k \nabla T) + \sum_i (-\Delta H_i \dot{\omega}_i), \quad (8)$$

where ρ – density;
c_p – specific heat capacity;
k – thermal conductivity;
$\dot{\omega}_i$ – reaction rate of species *i* weighted by its enthalpy of formation ΔH_i.

The concentration of each chemical species C_i (i.e. CH_4, CO, O_2) is governed by the reaction-advection-diffusion equation:

$$\frac{DC_i}{Dt} = \nabla \cdot (D_i \nabla C_i) + \dot{\omega}_i, \quad (9)$$

where D_i – diffusion coefficient of species i,
$\dot{\omega}_i$ – net production rate, Arrhenius-type [10].

In the case of a single global reaction, the production rate is modeled by

$$\dot{\omega}_i = A_i C_{\text{fuel}}^{n_i} C_{O_2}^{m_i} e^{-E_a/(RT)}, \quad (10)$$

where A_i – pre-exponential factor;
E_a – activation energy;
R – universal gas constant;
T – temperature.

By *fuel* we substitute the species being oxidized in each reaction (see Table 1).

The system is subject to the following boundary conditions: for temperature – homogeneous Neumann ($\nabla T \cdot \mathbf{n} = 0$) at walls; convective flux at the outlet and for species transport – Dirichlet boundary condition for inflow species concentrations; zero-flux Neumann condition at walls.

Table 1

Arrhenius parameters for the considered combustion reactions

Reaction	A_i, s^{-1}	E_a, $J \cdot mol^{-1}$	n_i	m_i
$CH_4 + 1.5O_2 \rightarrow CO + 2H_2O$	1.3×10^8	1.25×10^5	1	1.5
$CO + 0.5O_2 \rightarrow CO_2$	2.0×10^7	1.12×10^5	1	0.5
$H_2O + C \rightarrow CO + H_2$	4.5×10^5	8.5×10^4	1	0

The Arrhenius parameters for the considered reactions (primary combustion, secondary oxidation and gasification), based on Chemkin format [10], are given in Table 1.

The velocity equations are discretized by using finite volume techniques and currently implemented in Octave/Matlab environment. We use the voxel geometry, and it facilitates particle-wall collision detection. The temperature and species equations are discretized by finite difference techniques and currently implemented in Matlab/Octave/Python environment. In the section below we present some graphical results produced by our codes by commenting the obtained result and discussing their features.

Results and discussion

In [9] the geometry setting with obstacles has been introduced. The obstacle positions have been randomized. The solution of (1)-(7) has been executed. In Fig. 1 one can see that particles are deposited

at the outlet and near the obstacles. The obstacles' graph, used for various applications in [9], is on the left panel. Particle trajectories and deposition sites are on the right panel.

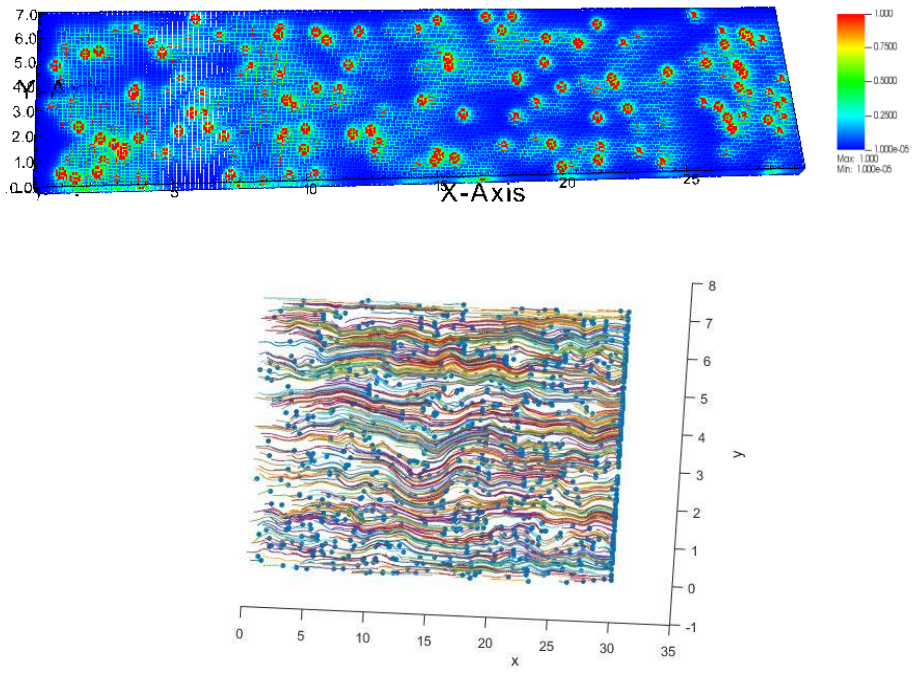

Fig. 1. **Flow through inhomogeneous porous domain with Lagrangian particle tracking**

In the present simulations, we have considered our full three-dimensional setting and track the particles in their no-collision mode – in Fig. 2 in the left panel there is no buoyancy or sedimentation effect and one can see the particles mostly obey the trajectories due to the drag force; in the right panel the combination with the sedimentation effect is observed with the non-dimensional gravity-describing parameter for the last term of equation (3) set to negative value.

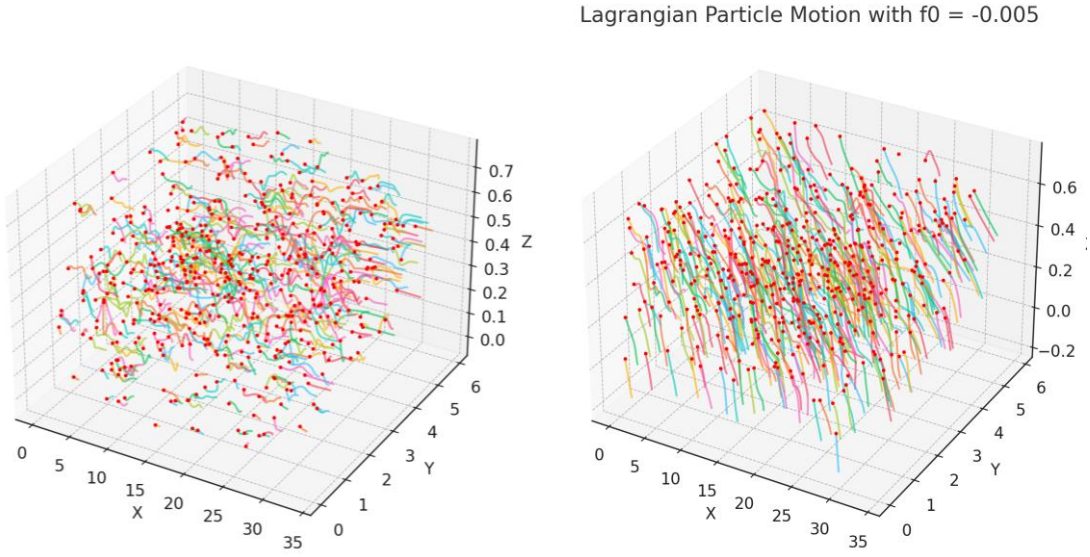

Fig. 2. **Lagrangian particle tracking and sedimentation effects**

Afterwards we extend our simulations with a very substantial feature for modelling the potential hot spots susceptible for auto-ignition – track the collisions and the deposition sites. In Fig. 3 one can see the results of our sample 1500-particles simulations (left panel) and six times more particles in the right panel, making the deposition effect more visible.

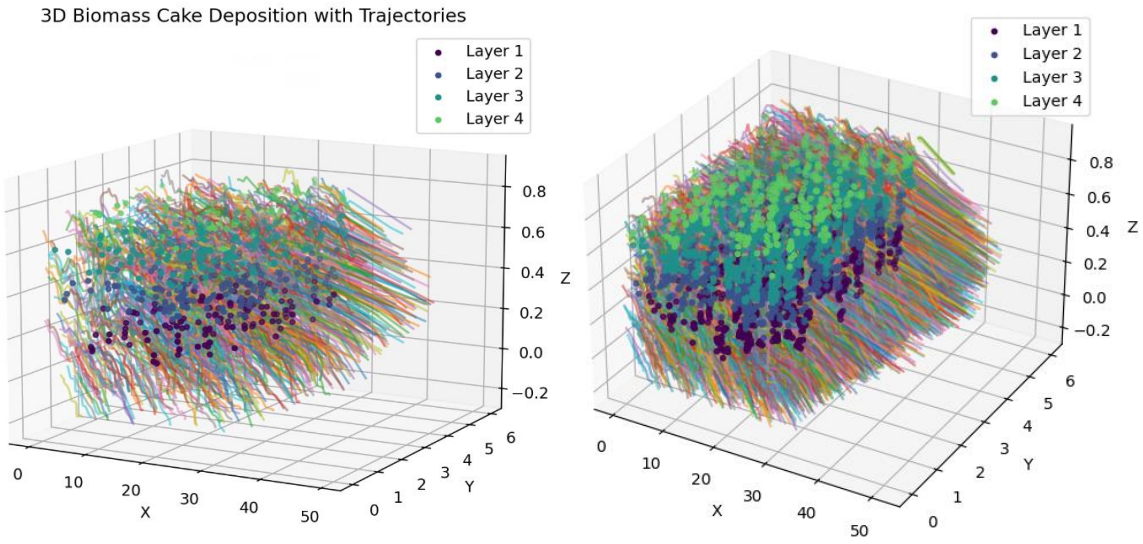

Fig. 3. **Lagrangian particle tracking with deposition sites**

One can see that some particles keep following the trajectories, while some are forming the deposition sites. We have emphasised different layers for geometrical reasons but at the same time other particle properties can be tracked this way.

Afterwards we consider deposition sites as local heat sources, dependent on the storage densities (in our model – how many particles get 'stuck' in the corresponding position) and solve the temperature and species equations (8)-(10). The corresponding source terms depend on data gathered on deposition sites (densities, locations and time moments of the deposition event). Fig. 4 shows the temperature change at time moments of particle collisions and eventually due to triggered chemical reaction.

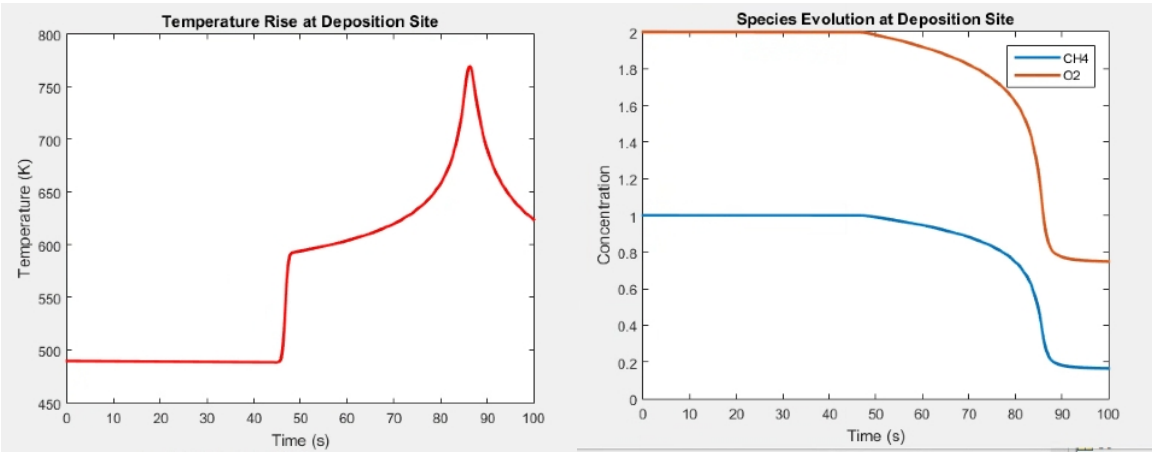

Fig. 4. **Temperature and concentration graphs at deposition sites**

On the left panel one can see a rapid increase exceeding 750 K due to exothermic chemical reactions. The species profiles (CH_4 and O_2, right panel) show the stoichiometric consumption, confirming thermal runaway at the deposition site. Afterwards we detect the zones of potential auto-ignition by observing the solutions of the combustion equations at several deposition sites at once. The diffusion effect takes place once the sites where both effects – the deposition and the triggered chemistry - are situated in a close radius (Fig. 5). Biomass auto-ignition occurs at around 400-600K depending on material type and other conditions [1]. Our results are also in line with the results in [2] and [7], where it is shown that repeated deposition of biomass particles can lead to gradual heating and potential thermal runaway.

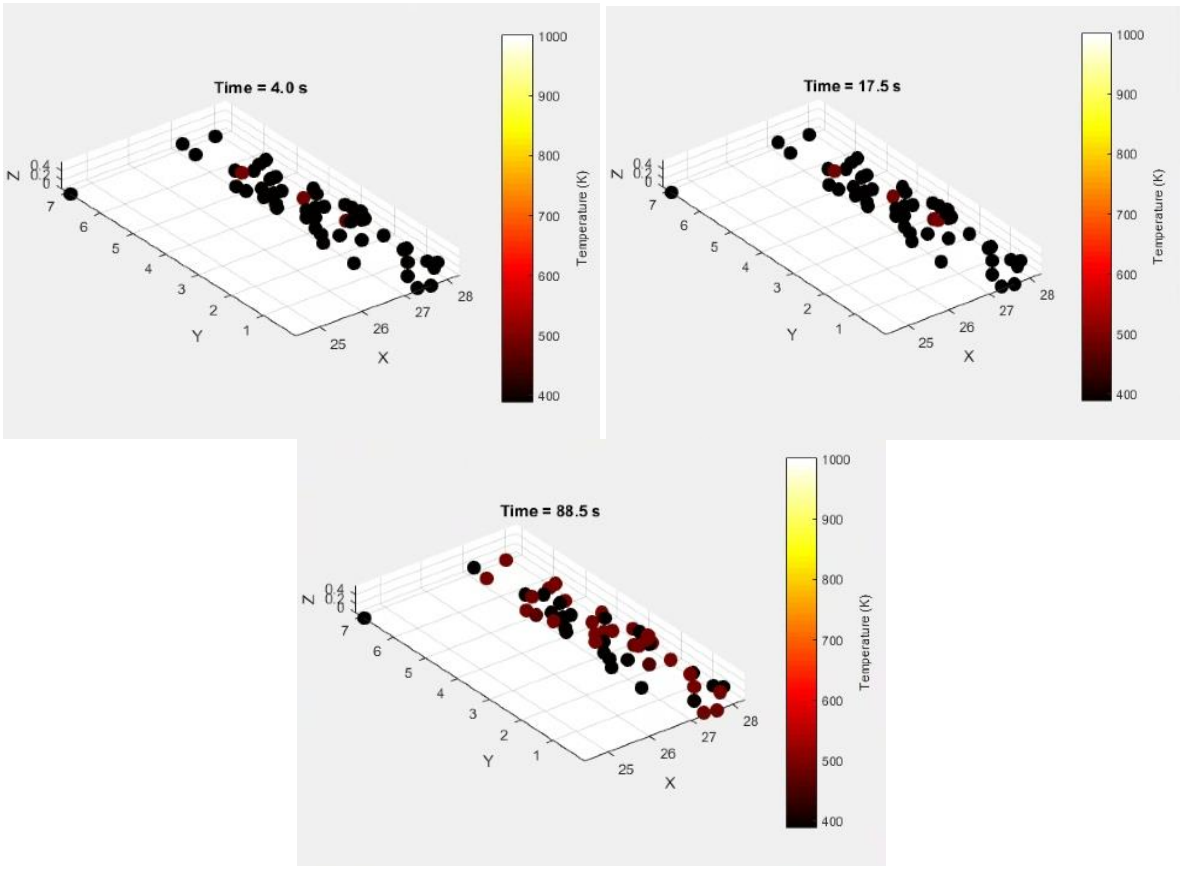

Fig. 5. **Zones of potential auto-ignition**

Since our models involve random obstacle allocations and randomized initial particle positions, our ability to repeat the entire simulation multiple times provides a statistically justified advantage in predicting the ignition risks. The framework is developed in a way that some of the geometry settings can be switched to deterministic, different velocity profiles or combustion modes can be used.

Present simulations do separate the treatment of several physical processes by decoupling the systems and approximate the complicated reaction mechanisms with general ones, however bringing more chemical reactions or deposition sites to the table makes the procedure much more computationally costly.

Conclusions

In this article we have described our working session where we have calculated the velocity field in the domain with randomly allocated obstacles and applied the particle tracking framework from our previous sessions for new, more sophisticated cases. We have observed the particle deposition sites and tracked different deposition densities and concluded that our model has a potential to predict auto-ignition zones in real-life applications. Hence, we have extended our models with temperature and species' equations and obtained our first results.

We have developed a localized ignition detection framework based on particle collision data, where each deposition site initiates a combustion model governed by Arrhenius kinetics. All deposition sites have been analyzed and one representative deposition site has been shown with the rise from an ambient level of 490 K to a peak of approximately 770 K and CH_4 and O_2 concentrations dropped significantly (by ~90%). A diffusion mechanism was added to simulate thermal interaction between neighbouring sites, and a visualization was built to track temperature rise and ignition zones over time.

This approach mirrors real-world scenarios in biomass silos and storage facilities, where clustered particle deposition can trigger localized heating and thermal runaway. Our method could potentially allow engineers to predict ignition thresholds, assess safety risks, and optimize system design to prevent deflagration and ensure operational reliability.

Our future endeavours shall involve more detailed chemistry description with might lead to necessity of better estimation of model parametrization and potentially more detailed discussed quantities' tracking on the particle level.

Author contributions

Conceptualization, U.S. and M.M.; methodology, U.S. and M.M.; software, U.S. and M.M.; validation, U.S. and M.M.; formal analysis, U.S. and M.M.; investigation, U.S. and M.M.; data curation, U.S. and M.M..; writing – original draft preparation, U.S. and M.M.; writing – review and editing, U.S. and M.M.; visualization, U.S. and M.M. All authors have read and agreed to the published version of the manuscript.

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