

# Implementation of Discrete Phase Model for Optimization of Chemical Looping Combustion Fuel Reactors

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## Abstract:

Chemical Looping Combustion (CLC) represents an alternative to conventional fuel combustion technologies due to its potential for high thermodynamic efficiency and inherent carbon dioxide capture. By employing circulating metal oxides as oxygen carriers (OC), CLC enables the conversion of solid, liquid, and gaseous fuels while avoiding energy-intensive CO<sub>2</sub> separation processes, thereby improving overall system efficiency. Due to the internal separation of exhaust gases and combustion products, this technology is particularly relevant for integration with renewable fuels, including biomass.

In practical applications, the operational efficiency of CLC systems is strongly influenced by the stable operation of the fuel reactor. Of particular importance are solid-phase transport, separation, and internal recirculation under complex flow conditions. Inefficient separation of oxygen carrier particles and unburned char leads to material losses and reduced conversion efficiency. Consequently, the effectiveness of gas–solid separation plays a decisive role in determining the overall performance of CLC reactors.

To address these challenges, various separator concepts have been proposed, and reactor designs have been continuously refined. A novel cuboidal CLC fuel reactor, described in Polish Patent PL243901B1, features an integrated inertial separator that enables the internal return of separated solids without the need for external separation devices. This compact configuration has the potential to reduce pressure losses, improve solids recirculation efficiency, and enhance the reactor thermal performance.

Before industrial implementation, advanced numerical simulations are essential for supporting efficiency-oriented design and optimization. Computational methods allow for systematic evaluation of design variants and operating conditions while significantly reducing the costs associated with experimental prototyping. In this context, the present paper discusses numerical approaches applied to the optimization of CLC systems, with particular emphasis on the Discrete Phase Model (DPM).

DPM is a Lagrangian CFD technique that resolves individual particle trajectories and accounts for momentum, mass, and heat transfer between the dispersed and continuous phases. This approach enables detailed analysis of particle residence time, separation efficiency, and thermal interaction with the gas phase—parameters that directly affect reactor efficiency. The novelty of this study lies in assessing the applicability of the DPM model for optimizing CLC reactor configurations, highlighting both its advantages and limitations for efficiency-driven design. The results indicate that DPM-based simulations provide a computationally efficient and physically consistent framework to support the optimization and scale-up of advanced CLC fuel reactor concepts.

## Keywords:

Chemical Looping Combustion (CLC); Optimization; Discrete Phase Model; Fuel Reactor, Negative CO<sub>2</sub> emissions.

# 1. Introduction

## 1.1. Background on Chemical Looping Combustion

Chemical Looping Combustion (CLC) has emerged over the last two decades as one of the most promising low-carbon combustion technologies, offering inherent CO<sub>2</sub> separation without the efficiency penalty associated with conventional post-combustion capture and compression schemes [1, 2]. In CLC, oxygen is supplied to the fuel via circulating metal oxides rather than directly by air, which prevents nitrogen from entering the fuel reactor and yields an exhaust stream composed mainly of CO<sub>2</sub> and H<sub>2</sub>O [3]. After condensation of water, a highly concentrated CO<sub>2</sub> stream is obtained, facilitating compression, transport, and storage and making CLC attractive for both retrofitted and newly built power and industrial plants. In addition, the process can be integrated with biomass and waste-derived fuels, enabling negative-emission concepts when combined with carbon capture and storage, as highlighted in recent reviews of biomass-fired CLC systems [4, 5].

The overall performance of CLC systems depends on the selection and behavior of oxygen carrier materials, typically based on oxides of nickel, iron, copper, or manganese, which differ in reaction kinetics, cyclic stability, tendency to sinter, and cost [6]. Iron-based carriers are particularly attractive due to their low cost, abundance, and environmental compatibility, despite their more complex redox stoichiometry and sometimes slower kinetics compared to nickel-based systems. For solid fuels such as coal and biomass, additional challenges arise from ash formation, alkali and chlorine interactions, and the need to ensure sufficiently intense mass and heat transfer between the gas phase and the reactive particles [3]. These effects strongly influence carrier deactivation, attrition, and agglomeration, and thus must be considered in both experimental and modeling studies aimed at the design of durable and efficient CLC units.

Alongside material development, a broad spectrum of reactor concepts has been proposed and demonstrated at lab-scale and pilot-scale, including dual bubbling fluidized beds, circulating fluidized bed (CFB) systems with external cyclones, and configurations integrated with reforming or hydrogen production [7-9]. Experience from scaling up CLC units from a few kilowatts to several megawatts shows that gas–solid hydrodynamics and solids circulation patterns in the fuel reactor are critical for achieving high fuel conversion, stable operation, and uniform temperature profiles. In particular, insufficient separation of oxygen carrier particles and unburned char can lead to material losses, reduced CO<sub>2</sub> capture efficiency, and operational instabilities, motivating the continuous refinement of separation devices and solids return systems. In this context, compact reactor layouts with integrated separation functionalities, such as novel cuboidal fuel reactors with internal inertial separators, have been proposed to reduce pressure drops, simplify the overall plant layout, and enhance solids recirculation efficiency within a single reactor envelope.

## 1.2. Modeling and Optimization Approaches for CLC Reactors

To support design, optimization, and scale-up of CLC systems, a wide range of modeling approaches has been developed at both system and reactor levels. At the system level, process simulation and thermodynamic analysis tools are commonly employed to evaluate plant-wide efficiency, heat integration, and CO<sub>2</sub> capture ratios for different CLC-based power cycles and industrial processes [10]. Such models are particularly useful for comparing alternative configurations, assessing the impact of operating conditions on net efficiency, and identifying optimal integration strategies with other units, but they typically rely on simplified reactor sub-models and do not resolve detailed gas–solid flow patterns.

At the reactor scale, one-dimensional and quasi-one-dimensional models based on two-phase theories (e.g., Kunii–Levenspiel), core–annulus concepts, or axial dispersion representations have been widely used to describe bubbling and circulating fluidized bed reactors in CLC applications [9, 11, 12]. These models capture axial profiles of conversion and temperature using averaged correlations for gas–solid contact, minimum fluidization velocities, solids circulation rates, and elutriation, which makes them computationally inexpensive and well-suited for extensive parametric studies and preliminary optimization. However, their inherently averaged nature limits their ability to represent complex three-dimensional geometries, internal separation devices, and localized flow structures that strongly affect particle residence times and separation efficiency in compact reactors [5, 13]. To address particle-scale phenomena such as oxygen carrier degradation, char combustion, and particle size evolution, particle population balance models and reduced-order combustion models have been coupled with these low-dimensional reactor descriptions, providing improved predictions of

particle size distributions, deactivation, and material losses while retaining relatively low computational cost interconnection [14]. In study [15], an order-reduced model, which can simultaneously simulate air reactor (AR) and fuel reactor (FR) as well as their heat/mass interaction via oxygen carrier (OC) circulation, was developed for a 10 MWth autothermal reactor for CH<sub>4</sub>-fueled chemical looping combustion (CLC). Initially, the gas-solid fluid dynamics, chemical reactions, and temperature/energy distributions within the two main reactors were discussed. The fluidization state of the entire setup meets expectations, achieving the combustion efficiency of 85.77% with a generally reactive Fe-based OC, and confirming the feasibility of autothermal operation of the reactor. Moreover, CFD simulation was employed to compare with the order-reduced model results, and a good agreement between the order-reduced simulation and CFD results was achieved. Nevertheless, these approaches still rely on strong spatial averaging and offer only indirect information on gas–solid hydrodynamics.

Another tool for building 1.5D models is presented in [16]. This work presents a 1.5D model of a fluidized-bed chemical looping combustion (CLC) developed using CeSFaMB, a comprehensive simulator of fluidized and moving-bed equipment. The presented model can calculate the effect of gas velocity in the fuel reactor on the fluidized-bed hydrodynamics and the CLC process kinetics.

Three-dimensional (3D) models, especially those based on Computational Fluid Dynamics (CFD), are a desirable tool for analyzing chemical looping combustion (CLC) systems because they allow for precise representation of complex hydrodynamics in space. Unlike 1D or 2D models, 3D simulations provide detailed insight into the spatial distribution of temperatures, gas concentrations, and solid-state flows and interactions, which is crucial for optimizing and scaling CLC technologies, especially for configurations with complex internal structures and separation zones.

Eulerian–Eulerian (two-fluid) models treat both gas and solid phases as interpenetrating continua and solve separate sets of conservation equations for each phase, supplemented by granular flow closures for solid stresses and interphase momentum exchange. This approach has been successfully applied to bubbling and circulating fluidized beds in CLC and related systems in [17-19], offering detailed fields of phase volume fractions, velocities, and temperatures; however, it often struggles to explicitly represent individual particle trajectories, inertial separation mechanisms, and fine-scale segregation in highly complex geometries.

In contrast, Eulerian–Lagrangian methods, and in particular the Discrete Phase Model (DPM) and its dense-phase extensions, track representative particles in a continuous gas field and naturally capture inertial separation, collisions with internal structures, and heterogeneous residence time distributions. DPM-based simulations have been shown to provide a favorable compromise between physical fidelity and computational cost compared with fully resolved CFD–DEM (Discrete Element Model) approaches, especially when focusing on reactor-scale phenomena such as internal solids circulation and gas–solid separation performance. The simulations demonstrated in [9] have proven the ability of CFD-DDPM (Dense Discrete Phase Model) to accurately capture the physics of the circulating fluidized bed-based CLC process at pilot scale, which can be extended to industrial scale projects.

Despite the extensive number of works on CLC modeling, relatively few studies offer a systematic comparison of the applicability, strengths, and limitations of different modeling approaches. From one-dimensional models to advanced CFD and CFD-DPM approaches, for the optimization of advanced fuel reactor concepts with integrated separation features. There is a particular need to clarify how each modeling strategy can contribute to design workflows aimed at improving gas–solid separation, particle residence time distributions, and thermal uniformity, while maintaining acceptable computational costs for iterative optimization and scale-up. The present paper addresses this gap by focusing on the implementation of a CFD–DPM framework for a novel construction of a fuel reactor, which is protected by patent no. PL243901B1. The analysis is complemented by comparisons with lower-order reactor models from the literature, thereby delineating the respective roles of reduced and advanced 3D models in the development and scale-up of advanced CLC fuel reactors.

## 2. Methods

### 2.1. CLC system modeling methods

In this work, several classes of modeling approaches commonly used for CLC fuel reactors are considered and compared in terms of their suitability for design and process optimization analyses. The comparative analysis of modeling approaches for CLC fuel reactors was carried out under the following assumptions and limitations.

First, only methods that are well documented in the peer-reviewed literature and have been applied to CLC or closely related gas–solid fluidized systems were considered, so highly speculative or purely conceptual approaches were excluded. Second, the comparison focused on aspects directly relevant to efficiency-oriented design and optimization of fuel reactors, namely the capability to represent gas–solid hydrodynamics, particle residence time, separation performance, and thermal behavior, as well as the associated computational cost and ease of integration into engineering workflows.

Based on the methodological analysis described above, the different modeling approaches for CLC fuel reactors were subsequently compared using a unified set of criteria, and the outcomes of the analysis are presented in the Results section of Table 2. Using these common benchmarks and tabular form in the Results section allows a transparent assessment of their relative strengths and limitations and provides a consistent basis for selecting CFD-DPM as the primary approach for the present study.

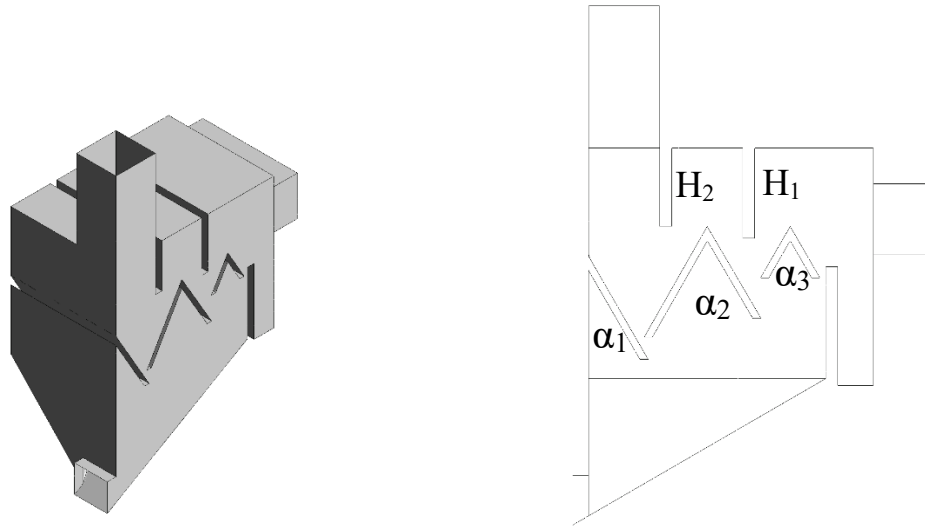
### 2.2. DPM-CFD computational model

The computational model combines an Eulerian description of the gas phase with a Lagrangian tracking of the solid particles within the patented CLC fuel reactor equipped with an integrated inertial separator. The gas flow is resolved using steady-state Reynolds-Averaged Navier–Stokes equations supplemented by an energy equation to capture non-isothermal conditions in the separator domain.

Turbulence is modeled with the SST  $k$ - $\omega$  turbulence model, ensuring an accurate representation of recirculation zones and near-wall phenomena in the complex baffle–bulkhead system. The discrete phase is represented by oxygen carrier and char particles injected at the inlet and tracked in a two-way coupled DPM framework, which accounts for momentum and energy exchange between phases.

The 3D computational domain of the patented reactor (PL243901B1) was discretized using the ANSYS Meshing 2026 R1 software package. The high-quality polyhedral mesh was created, complemented by inflation layers along solid walls with a transition ratio of 0.272, ensuring a smooth volumetric transition from the dense near-wall elements to the polyhedral cells. Mesh independence was verified using the Grid Convergence Index methodology to ensure that key hydrodynamic and thermal indicators are insensitive to further grid refinement.

The geometry in 3D and 2D of the particle separator located in the volume of the fuel reactor is shown in Figure 1.



**Figure 1.** The view of particle separator geometry in 3D – on the right and 2D – on the left, where the modified collision bulkheads ( $H_1$  and  $H_2$ ) and the baffle inclination angles ( $\alpha_1$ ,  $\alpha_2$ ,  $\alpha_3$ ) are marked.

The geometric parameters of the particle separator in the fuel reactor were analyzed, as its design directly influences the separation efficiency of the fuel and oxygen carrier particles circulating in the fluidized bed. The set of analyzed cases is presented in Table 1, along with the individual dimensions of the separator components.

**Table 1.** Summary of the analyzed cases

No. Case	$\alpha_1$ [°]	$\alpha_2$ [°]	$\alpha_3$ [°]	H1 [mm]	H2 [mm]
C1	50	50	25	38	38
C2	50	50	25	20	20
C3	60	60	30	38	38
C4	60	60	30	33	38

Hydrodynamic boundary conditions are adopted from the validated cold-flow model described and validated in [20], including inlet velocity and pressure based on laboratory measurements, defined pressure outlets at the solids chute and flue-gas exit, and no-slip conditions at all remaining walls. This setup enables consistent evaluation of separator performance across operating regimes.

### 3. Results and discussion

#### 3.1. Summary of analyzed modeling methods

The summary of the analyzed modeling methods available in the literature is presented in Table 2.

**Table 2.** Summary of analyzed modeling methods

Approach	Hydrodynamics resolution	Typical implementation in CLC literature	Advantages	Limitations	Ref.
1D / 1.5D reactor models (Kunii–Levenspiel,	Axial profiles, cross-sectionally averaged	Fast assessment of operating conditions, simple optimizations	Very low computational cost, easy integration with	No 3D information, limited ability to analyze separator geometry	[12, 16, 17, 21]

Approach	Hydrodynamics resolution	Typical implementation in CLC literature	Advantages	Limitations	Ref.
core annulus, ADM)			system-level analysis		
PBM + reduced-order combustion models	Averaged hydrodynamics, particle size distributions	Analysis of oxygen carrier deactivation, char combustion, material losses	Better representation of solid-phase evolution than pure 1D models	Strong spatial averaging, no explicit particle trajectories	[14, 15, 22]
CFD Euler–Euler (TFM)	Full 3D for both phases treated as continua	Bubbling/CFB reactors, general hydrodynamics, scale-up studies	Detailed fields of volume fraction, velocity, and temperature	Complex closure models, high mesh cost, challenges for inertial separation in non-standard geometries	[17, 23, 24]
CFD–DPM / Dense DPM (Euler–Lagrange)	3D gas field + trajectories of representative particles	Analysis of separation, recirculation, separator design, residence time	Good compromise between particle-scale detail and computational cost, natural description of inertial separation	Limitations for very dense beds, need for calibration of collision and coupling models	[20, 24, 25]
DEM or hybrid CFD–DEM	Fully resolved motion and collisions of individual particles	Fundamental studies, small scales, and validation of simplified models	Most detailed description of particle dynamics	Very high computational cost, limited practicality for reactor-scale optimization	[26]

According to the above list, low-dimensional reactor models (1D and quasi-1D two-phase models) are present as a reference for fast parametric studies and for estimating global indicators such as fuel conversion, temperature profiles, and overall solids circulation. These approaches provide very low computational cost and are convenient for preliminary screening of operating conditions and design variants. Still, they rely on strong spatial averaging and therefore cannot resolve complex three-dimensional flow structures, internal separation zones, or detailed particle residence time distributions in compact fuel reactors.

Next, particle population balance models (PBM) and reduced-order combustion models are considered as intermediate-fidelity tools that enrich low-dimensional descriptions with information on particle size distributions, oxygen-carrier degradation, and char conversion. While these methods improve the representation of the evolution of the solid phase, they still treat gas–solid hydrodynamics in a highly averaged way and only indirectly capture phenomena such as inertial separation or localized recirculation loops.

Three-dimensional multiphase CFD approaches are therefore introduced in the literature as high-fidelity alternatives. The Eulerian–Eulerian (two-fluid) and Eulerian-Lagrangian models resolve detailed fields of gas and solids volume fractions, velocities, and temperatures, but require complex closure relations for granular

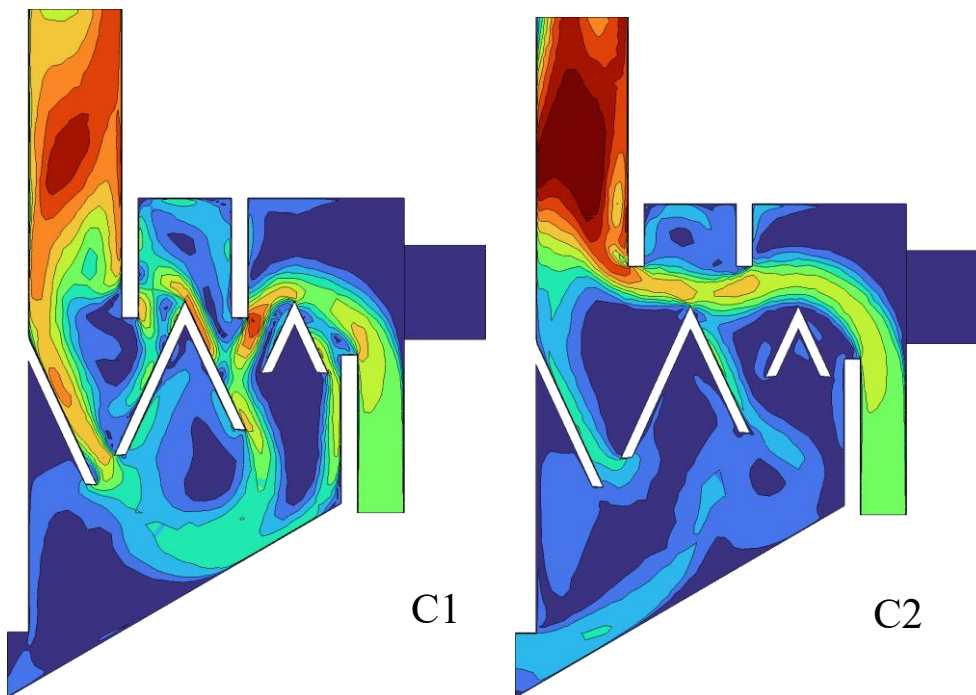
stresses and are less suited to explicit analysis of individual particle trajectories and separator performance in intricate geometries [27].

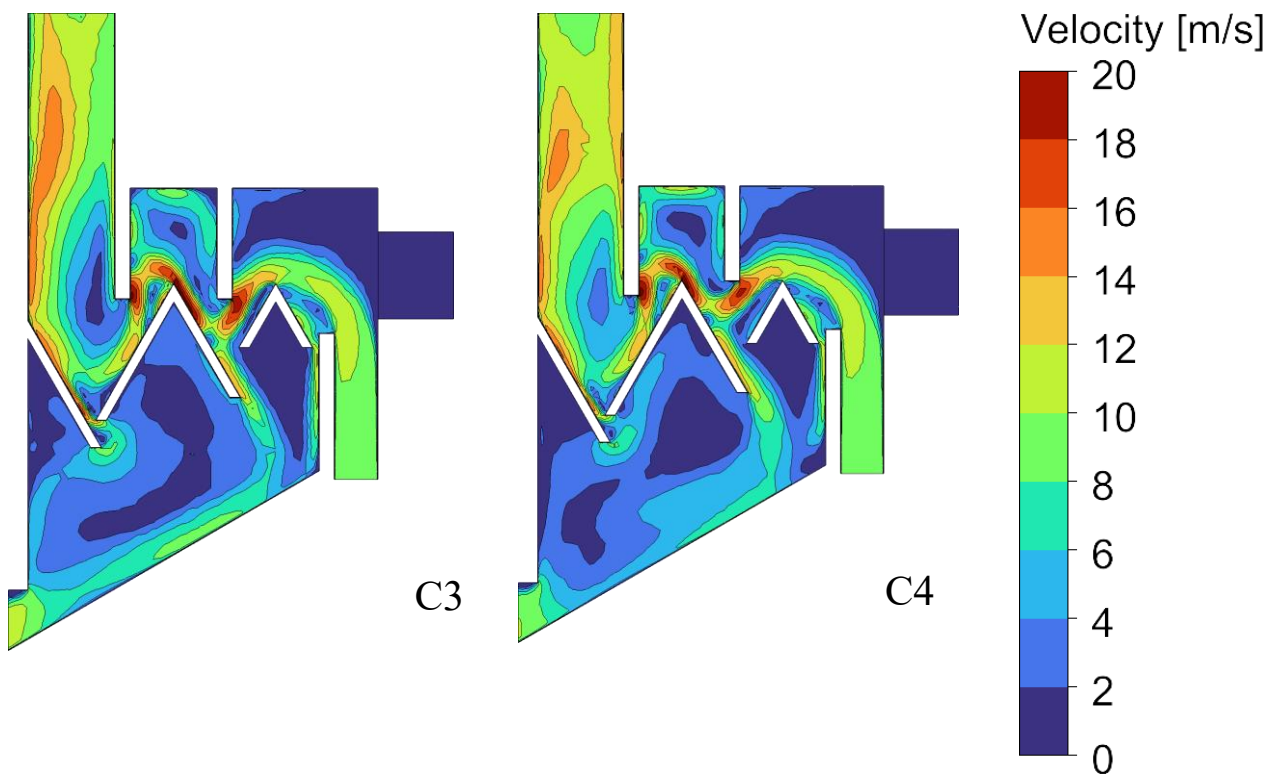
### 3.2. CFD-DPM simulation results

CFD-DPM analyses were performed using Ansys Fluent 2026 R1 version. Figure 2 shows the velocity fields for the analyzed particle separator geometries.

In all simulated cases, the gas velocity field reveals the formation of intense recirculation zones in the vicinity of the collision bulkheads H1 and H2, which promote lateral deflection of the particle-laden stream towards the internal separation chamber. For cases C1 and C3, characterized by higher baffle inclination angles, the recirculation cells are more compact and closer to the separator entrance, whereas in C2 and C4 the weaker deflection leads to a more direct gas–solid path towards the outlet.

The DPM results indicate that particle trajectories are strongly affected by both the baffle angles ( $\alpha_1$ – $\alpha_3$ ) and the vertical positions of bulkheads H1–H2. For configurations C1 and C3, a larger fraction of oxygen carrier and fuel particles is redirected towards the return duct, resulting in an increased residence time within the separator volume and a reduced fraction of solids escaping with the flue gas. In contrast, configurations with shortened bulkheads (C2) or reduced vertical offset (C4) exhibit a higher proportion of particles entering the upper outlet region, which corresponds to lower internal separation performance.





**Figure 2.** The velocity fields for the analyzed particle separator geometries

## 4. Conclusions

The study has reviewed key modeling strategies for Chemical Looping Combustion fuel reactors, from 1D/1.5D reactor models and population balance approaches to high-fidelity multiphase CFD and CFD-DPM methods, highlighting their suitability for design and optimization. By applying a unified set of criteria, the respective roles of reduced-order and advanced 3D models in CLC technology development have been clarified.

On this basis, a CFD-DPM model was implemented for a patented fuel reactor with an inertial separator (PL243901B1) and used to analyze several cases of separator geometries. The results show that the Eulerian–Lagrangian description can capture inertial separation, internal recirculation zones, and particle residence time distributions with a level of detail not achievable by low-dimensional models alone. The obtained results demonstrate that relatively small modifications of separator geometry significantly influence particle separation efficiency. Configurations with increased baffle inclination and appropriately positioned bulkheads offer the best compromise between enhanced internal recirculation and limited hydraulic resistance, supporting the concept of compact fuel reactors with integrated separation.

Overall, CFD-DPM is confirmed as an effective and computationally tractable tool for the design and optimization of CLC fuel reactors and separators. In engineering practice, it should be combined with faster low-dimensional and system-level models for plant-wide analysis, while future work will focus on extending the present cold-flow framework to reactive and hot conditions.

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