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Numerical Simulation of Airflow and Iron Particle Behavior in the MC2 Reactor

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Abstract. This research presents a comprehensive numerical simulation of air flow and iron powder injection in a Metal Cyclonic Combustor (MC²) using ANSYS Fluent 2024 R1. The main objective is to analyze the flow pattern and particle dynamics in a two-phase system subjected to swirling conditions. The geometry of MC² is designed with two tangential air inlets and a central iron powder injector, aiming to enhance efficient mixing and stable combustion. Air is introduced at a velocity of 2.5 m/s and preheated to 1073 K, while iron particles with a diameter of 10 microns are injected at a mass flow rate of 0.76 g/s. To accurately capture the turbulent air flow, the k-ω SST turbulence model is used, while the Discrete Phase Model (DPM) is used to track the motion of iron particles in the flow field. The simulation results reveal the formation of strong swirling eddies that effectively distribute iron particles throughout the combustor, enhancing the possibility of uniform combustion. The maximum velocity recorded reaches approximately 61,970 m/s, predominantly concentrated near the inlet and upper regions of the chamber, which indicates a high-speed entry and the influence of turbulent mixing in these zones. The time range is around 0 to 0.06345 seconds, but most of the relatively short particle times range between 0 and 0.03 seconds. Therefore, the interaction between swirling air and particle dispersion is found to be critical in achieving efficient energy release from the metal fuel.

1 Introduction

The urgent global challenge to reduce greenhouse gas emissions and achieve sustainable energy systems has accelerated the search for alternative energy carriers. In general,

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renewable energy will be able to improve sustainable economic development, environmental challenges, society role, economic growth, and international support [1]. Among various candidates, metal powders, particularly iron, have emerged as promising solid fuels due to their high energy density, carbon-free combustion, and full recyclability [2][3].

Iron powder combustion offers several advantages over traditional hydrocarbon fuels: it produces no CO_2 emissions during combustion, generates stable energy output, and can be regenerated through reduction processes powered by renewable energy sources. Furthermore, the abundance of iron on Earth and its safety in storage and transport compared to hydrogen or fossil fuels position it as a viable candidate for the future of sustainable energy systems [4].

To harness these advantages, innovative combustion technologies such as the Metal Cyclonic Combustor (MC^2) have been developed. The MC^2 itself is characterized by a combustion chamber with a diameter of 60.8 mm and a height of 187 mm, featuring an air inlet with a diameter of 4 mm and an outlet with a diameter of 16 mm, providing a compact yet efficient configuration for high-performance combustion processes. Swirling flows within such combustors enhance flame stabilization, promote homogeneous particle-air mixing, and improve residence time, leading to more efficient combustion [5][6]. Maintaining high swirl numbers within the combustor facilitates the formation of strong recirculation zones that are vital for sustaining stable metal flames.

Computational Fluid Dynamics (CFD) has emerged as an indispensable tool for studying and optimizing these complex systems. The use of models such as k-ω SST turbulence combined with Discrete Phase Model (DPM) allows for accurate prediction of both gas-phase turbulence and particle trajectories under swirling conditions [7][8]. Recent developments have focused on optimizing key operational parameters to ensure complete combustion and minimal emissions. In the context of MC^2 systems, specific conditions such as air injection velocity of 2.5 m/s, preheating of air to 1073 K, iron powder flow rate of 0.76 g/s, and particle diameter of 10 microns have been employed to achieve optimal combustion performance. These parameters are critical to achieving rapid ignition, minimizing particle agglomeration, and ensuring uniform flame propagation across the combustor volume. The particle size greatly influences combustion behavior, where smaller particles (such as 10 microns) ensure faster heating and ignition but also require careful management to avoid excessive vaporization [9]. Preheating the carrier air to high temperatures like 1073 K significantly lowers the ignition delay and enhances the stability of the iron flames, while maintaining a moderate air velocity (2.5 m/s) ensures effective mixing without excessive dispersion of the powder [10]. Consequently, a comprehensive understanding of the velocity, thermal environment, and discrete phase interactions in such systems is vital for advancing zero-carbon, high-efficiency metal fuel technologies. This study focuses on numerically investigating iron powder flow and particle track, under these specified operational parameters and geometric dimensions, to provide insights for future large-scale applications.

Through the CFD analysis, it is observed that the swirling motion generated within the MC^2 chamber creates a strong central recirculation zone, significantly affecting the trajectory and residence time of the iron particles. The iron particles introduced into the combustor follow a helical path, gradually moving towards the combustion center where they experience intense thermal conditions leading to rapid ignition. The swirling flow ensures that particles remain suspended longer within the high-temperature core promoting complete combustion and reducing unburnt residues. Moreover, the combination of the high preheat temperature and controlled inlet velocity helps maintain a uniform dispersion of particles, minimizing agglomeration and ensuring that the particle combustion is spatially distributed throughout the chamber volume. The design parameters of the combustor, particularly the relatively small inlet (4 mm) and larger outlet (16 mm), are crucial in maintaining the necessary pressure drop and flow field structure, thereby supporting the effective movement and combustion of iron particles inside the chamber.

2 Methodology

This research presents a comprehensive numerical simulation of air flow and iron powder injection in a Metal Cyclonic Combustor (MC^2) using ANSYS Fluent 2024 R1. To investigate the Airflow and Iron Particle Behavior in a Metal Cyclonic Combustor (MC^2), a comprehensive numerical approach based on Computational Fluid Dynamics (CFD) simulations is used. The methodology is designed to accurately capture the swirling flow characteristics, the interaction between the carrier air and the injected iron particles, and the distribution of temperature under the specified operating conditions. This approach aligns with previous studies that have utilized CFD to analyze swirling particle-laden flows in combustor system.

This section details the steps undertaken, including the geometry and mesh generation, boundary conditions definition, physical models employed, simulation settings, and post-processing procedures, to ensure a reliable and robust representation of the MC^2 system. Figure 1 is a schematic diagram as the flowchart of this research which depicts the step of the method of research.

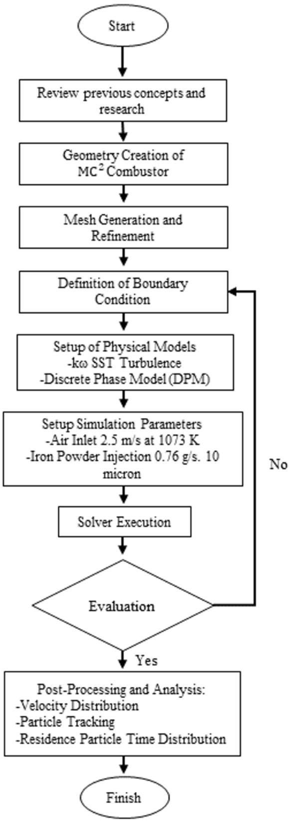

Fig. 1. Flowchart Research Method.

2.1 Geometry and Mesh

The initial phase involved developing a precise 3D model of the cyclonic combustor using Autodesk Invertor Professional, the combustor geometry was defined with a combustion chamber diameter of 60.80 mm, height of 172 mm, inlet diameter of 4 mm, and outlet diameter of 16 mm (Figure 2), accurately replicating experimental setups reported in prior studies. This was followed by generating a high-quality computational mesh using ANSYS Meshing, ensuring sufficient resolution near critical regions such as the inlet, outlet, and wall boundaries. A mesh independence study was conducted, comparing simulation outputs across progressively refined meshes to ensure solution stability and accuracy, consistent with the guidelines provided in recent CFD studies on combustion systems [11], [12].

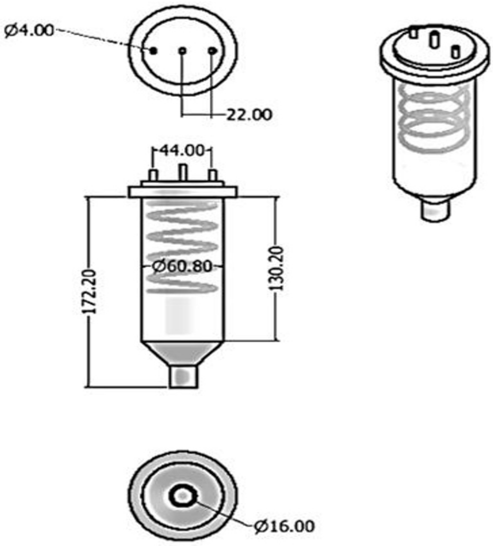

Fig. 2. Drawing Geometry Metal Cyclonic Combustor.

The computational domain is discretized using structured hexahedral meshes with local refinements near the inlet, outlet, and wall regions to capture flow gradients effectively. A mesh independence study is performed, resulting in a final mesh comprising approximately 1.2 million cells. Table 1 below is the explanation of meshing setup.

Table 1. Meshing Setup.

Parameter	Value	Description
Mesh type	Structured hexahedral	Hexa mesh with local refinement
Total number of cells	~1.2 million	After mesh independence study
Solver Type	Pressure-based	Steady-state solution
Pressure-velocity coupling	SIMPLE	Scheme used
Residual convergence criteria	10^{-5}	For all equations
Discretization schemes	Second-order upwind	Momentum, energy, turbulence

2.2 Definition of Boundary Conditions and Operating Parameters

The inlet conditions were set with a uniform air velocity of 2.5 m/s, and the air was preheated to 1073 K to simulate realistic combustion conditions as reported in recent studies [13]. The outlet was defined as a pressure outlet at atmospheric pressure, while the chamber walls were set as no-slip boundaries with adiabatic or fixed temperature conditions, depending on the wall segment, to accurately model heat transfer. Table 2 describes the boundary conditions and operating parameters.

Table 2. Boundary Condition and Operating Parameter of Simulation.

Parameter	**Value**	**Description**
Inlet air temperature	1073 K	Preheated air
Inlet air velocity	2.5 m/s	Injection speed
Iron powder flow rate	0.76 g/s	Mass flow rate of particles
Particle diameter	10 microns	Monodisperse particles
Chamber diameter	60.80 mm	Combustion chamber
Chamber height	173 mm	Combustion chamber
Inlet diameter	4 mm	Tangential inlet
Outlet diameter	16 mm	Outlet exhaust
Turbulence model	k-ω SST	RANS turbulence modelling
Discrete Phase Model (DPM)	Activated	Tracking particle movement

Iron powder with a mean particle diameter of 10 µm was injected using the Discrete Phase Model (DPM), and particle properties such as density, specific heat, and melting point were carefully assigned based on experimental data from the literature [13], [14]. The realizable k-ω turbulence model was selected due to its well-demonstrated capability in simulating swirling flows and recirculation regions within combustors [15].

2.3 Simulation Settings

The numerical simulation of iron powder combustion in the MC^2 system was conducted using ANSYS Fluent with a pressure-based solver and the SIMPLE (Semi-Implicit Method for Pressure-Linked Equations) algorithm for pressure-velocity coupling, which has been widely adopted in recent CFD studies to ensure robust and efficient convergence under reacting multiphase flows[11]. The spatial discretization employed second-order upwind schemes for momentum, energy, and turbulence equations, which significantly improves accuracy and reduces numerical diffusion, especially under swirling and recirculating flow conditions. To accurately resolve near-wall and core flow structures, the k-ω SST turbulence model was applied, providing superior predictions in swirling combustor configurations [12].

The Discrete Phase Model (DPM) was used to track the iron powder particles, considering drag force, turbulent dispersion, and heat transfer between the gas and particle phases. This approach has been validated in multiple recent studies, demonstrating its capability to capture detailed particle dynamics, such as trajectory, residence time, and vaporization behavior. Convergence criteria were set at 10^{-5} for residuals of continuity, momentum, energy, and turbulence quantities, and the DPM iteration limit was carefully tuned to ensure stable and accurate particle tracking.

2.4 Post-processing

Post-processing was conducted using ANSYS CFD-Post. Detailed analysis of flow fields included examining velocity magnitude contours, streamlines, vorticity patterns, and swirl intensity, providing insights into the formation of recirculation zones and the overall aerodynamic behavior of the combustor. For the particle phase, the results were evaluated for particle dispersion patterns, wall impingement locations, and residence time distributions, enabling a deeper understanding of how the flow field influenced combustion behavior. The results were validated against published numerical and experimental data where available, ensuring reliability and robustness.

3 Result and Discussion

3.1 Velocity Field Analysis of Steel Particle Flow in the Combustion Chamber

Based on the simulation results presented in the Figure 3, the velocity distribution of the steel particles inside the combustion chamber exhibits significant variation across different regions, reflecting the complex flow behavior and interaction with the chamber geometry. The maximum velocity recorded reaches approximately 61,970 m/s, predominantly concentrated near the inlet and upper regions of the chamber, which indicates a high-speed entry and the influence of turbulent mixing in these zones. In contrast, the lower section of the chamber shows a gradual reduction in velocity, demonstrating energy dissipation as the flow progresses toward the outlet.

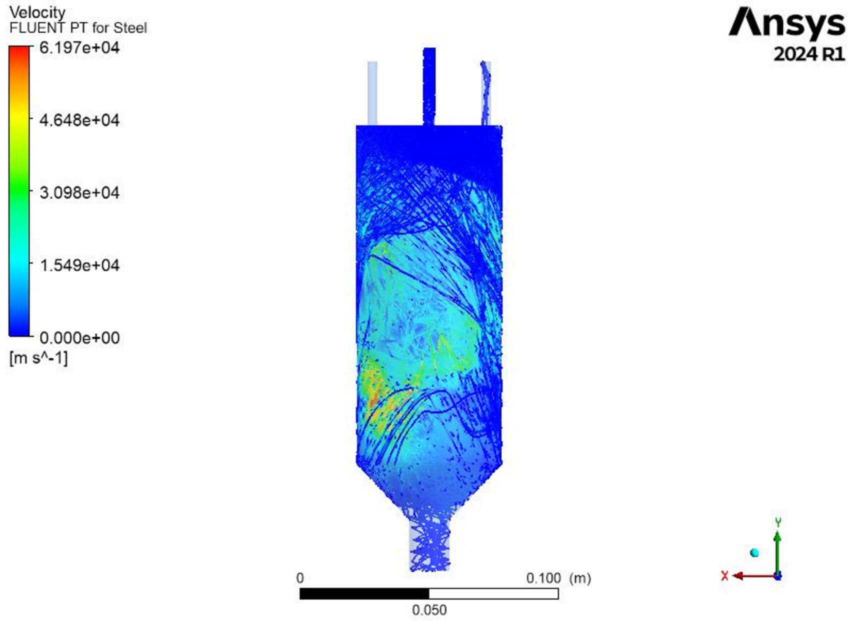

Fig. 3. Velocity Distribution.

The velocity contours reveal the development of recirculation zones and swirling patterns inside the chamber, which play a critical role in particle residence time and distribution. These flow structures enhance mixing and contribute to the uniform distribution of particles, ensuring effective process performance. The trajectories of the particles suggest that after entering the chamber at high speeds, they experience a complex path characterized by deceleration, redirection, and dispersion, influenced by the chamber design and boundary conditions. Additionally, the simulation confirms that the chosen configuration promotes effective momentum transfer and mixing, which are crucial for optimizing particle interactions and improving overall system efficiency. The combination of high inlet velocities and well-developed flow patterns provides valuable insights into the hydrodynamic behaviour of the system, highlighting areas where design modifications could further improve performance. Overall, the velocity analysis from the simulation validates the setup and provides an essential foundation for further investigation of particle time, pressure distribution, and detailed residence time analysis, supporting the main objectives of the research.

3.2 Particle ID Track

The particle track simulation illustrates the distribution and motion of steel particles within the combustion chamber, which has a diameter of 60.80 mm, a height of 172 mm, an inlet diameter of 4 mm, and an outlet diameter of 16 mm (Figure 4).

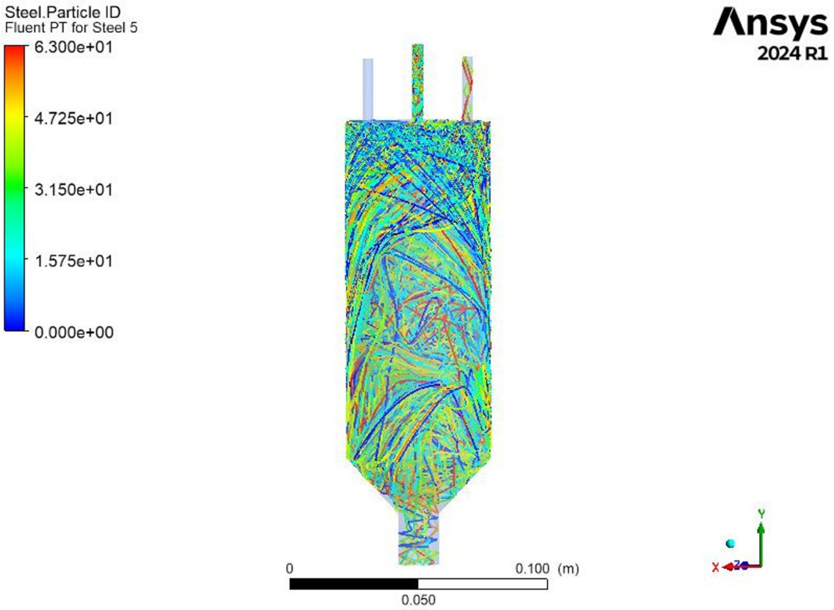

Fig. 4. Particle ID Track.

Based on the particle ID legend, the maximum recorded value reaches approximately 63 (6.300e+01), which indicates zones of high particle presence and interaction. The particles enter the chamber through the inlet at the top, and as they interact with the swirling flow field, they follow complex helical and recirculating paths throughout the chamber volume. The flow characteristics induce particle dispersion that covers almost the entire chamber cross-section, with a particularly intense concentration near the upper part where the inlet jet generates strong momentum. This distribution pattern is crucial in understanding the particle residence time and identifying zones with potential particle accumulation or wall collisions. The dense particle trajectories near the walls suggest areas where erosion or deposition may occur, which could impact system performance and durability. Additionally, the even spread of particle motion throughout the chamber indicates effective mixing, which is essential for optimizing reactions or separation processes inside the device.

3.3 Particle Time Analysis

Based on the simulation results obtained using ANSYS Fluent 2024 R1, the distribution of Particle Time for steel particles inside a vertical reactor or vessel has been visualized (Figure 5). The simulation results present a time range from 0 to approximately 0.06345 seconds. This distribution provides important insights into the particle flow behaviour within the system.

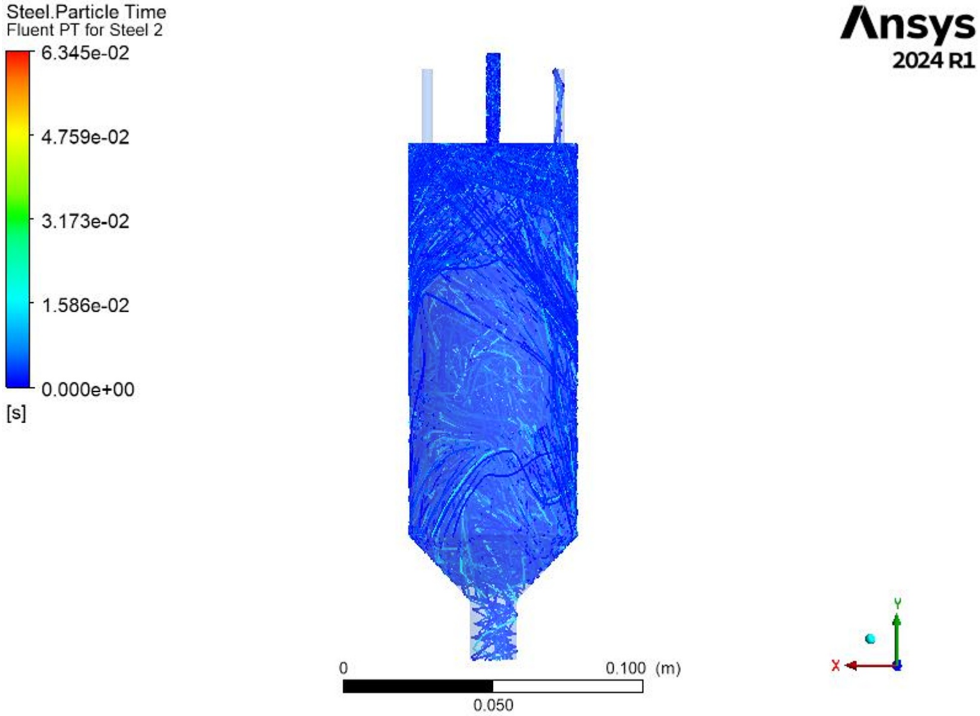

Fig. 5. Particel Time Analysis.

From the colors contour shown in the image, it can be observed that most of the vessel area is dominated by dark blue to light blue shades, indicating relatively short particle times ranging between 0 and 0.03 seconds. Only a small portion of the domain shows longer residence times, around 0.06 seconds, visible in the green to yellow-red regions. This phenomenon indicates that most particles pass through the system quickly, while a small fraction experiences flow retardation, resulting in longer residence times.

In general, the Particle Time distribution reveals a significant variation in particle behavior. At the bottom section of the vessel, particle times are very short, indicating that particles are efficiently directed toward the outlet without much obstruction or turbulence. In contrast, the middle to upper sections of the vessel shows larger particle times, suggesting that particles encounter more complex flow interactions, including potential recirculation zones or turbulent regions, which increase their residence time.

The distribution pattern of Particle Time also highlights areas with efficient particle transport and regions with potential stagnation or particle accumulation. This information is critical because particle residence time is closely linked to process efficiency, mixing quality, and possible operational issues such as build up or wall erosion due to uneven particle movement.

In conclusion, the Particle Time analysis in this simulation successfully reveals key characteristics of particle dynamics within the vessel. Most particles exhibit relatively short residence times, particularly along the main paths toward the outlet, while some areas show longer residence times due to complex flow interactions. These findings can serve as a foundation for evaluating potential design improvements or process optimizations to achieve a more uniform particle time distribution and meet desired operational goals.

4 Conclusion

The simulation results provide a comprehensive understanding of steel particle behaviour within the combustion chamber, focusing on velocity distribution, particle tracking, and residence time analysis. The velocity field analysis reveals high-speed particle entry with significant flow variations, including recirculation zones and swirling patterns that enhance mixing and system efficiency. The maximum velocity recorded reaches approximately 61,970 m/s, predominantly concentrated near the inlet and upper regions of the chamber, which indicates a high-speed entry and the influence of turbulent mixing in these zones. Particle tracking indicates a widespread and complex motion pattern throughout the chamber, highlighting effective dispersion and identifying regions of potential erosion or accumulation near the walls. Meanwhile, the particle time analysis demonstrates that most particles have short residence times, especially near the outlet, while longer durations occur in areas with recirculation or flow complexity. The time range is around from 0 to 0.06345 seconds but most of relatively short particle times ranging between 0 and 0.03 seconds, so only a small portion of the domain shows longer residence times, around 0.06 seconds. Collectively, these findings validate the chamber's design and offer valuable insights for optimizing performance, improving mixing uniformity, and minimizing operational risks such as erosion or build up. Overall, the findings of this study provide valuable insights into the design and optimization of metal fuel combustion systems, which offers a promising pathway towards sustainable and recyclable energy solutions utilizing iron powder combustion.

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