Numerical Simulation of Plastic Pyrolysis*

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Abstract

Pyrolysis of plastic waste for base chemical production is a pivotal technology for closing the carbon cycle and advancing sustainable energy transition. This work presents an overview of research activities conducted at the Institute for Technical Chemistry (ITC) at KIT, focusing on the simulation of plastic pyrolysis to develop efficient and cost-effective recycling technologies. A key objective of this research is to elucidate the physicochemical behavior during pyrolysis through high-fidelity numerical simulations, leveraging high-performance computing resources. These simulations provide fundamental insights essential for process design and optimization. Several ongoing studies are discussed, systematically spanning from fundamental single-particle analyses to fully resolved laboratory-scale fluidized bed reactors. These investigations evaluate the impact of key operating conditions and reactor design parameters on pyrolysis performance, demonstrating how numerical simulations can streamline and optimize the design process.

1 Introduction

Currently, only about 9% of global plastic waste—approximately 350 million tons annually—is recycled. The remaining 90% is either landfilled, incinerated, or released into the environment, leading to severe pollution problems [1, 2]. The low recycling rate stems from the limitations of conventional mechanical recycling, which can only process highly pure plastic waste. In contrast, chemical recycling via pyrolysis reverses the polymerization process used in plastic production, enabling the recycling of mixed and contaminated plastics. During pyrolysis, plastic polymers are thermally broken down into petrochemical feedstocks, which can then be used to manufacture new plastics, creating a closed-loop recycling system. As shown in Fig.1, plastic waste is converted into pyrolysis oil, which can be further refined into plastic pellets and new plastic products.

The pyrolysis process is governed by numerous parameters, including reactor temperature, flow and heating conditions, residence time, particle size, and catalyst use. Additionally, the reactor type, geometry, and dimensions significantly influence pyrolysis performance. Given this complexity, experimental investigations covering the full range of operating and design parameters are highly challenging and time-intensive. Consequently, prior research on plastic pyrolysis has primarily relied on small-scale experiments using milligram to gram quantities of plastic. These studies have provided critical data on reaction kinetics, pyrolysis product distribution, and material thermodynamics, demonstrating the technology's potential for plastic recycling at the laboratory scale. However, the interplay of multi-scale and multi-physical phenomena—coupled with the vast parameter space—makes precise control over product yield difficult. Furthermore, findings from lab-scale experiments often fail to translate directly to industrial-scale pyrolysis plants due to substantial differences in reaction and flow conditions. Thus, further optimization is essential to enhance scalability, energy efficiency, product yield, and economic viability for real-world applications.

To address this challenge, we employ numerical simulations to investigate multiphase reactive flows, enabling a fundamental understanding of plastic pyrolysis at unprecedented resolution. Unlike experimental

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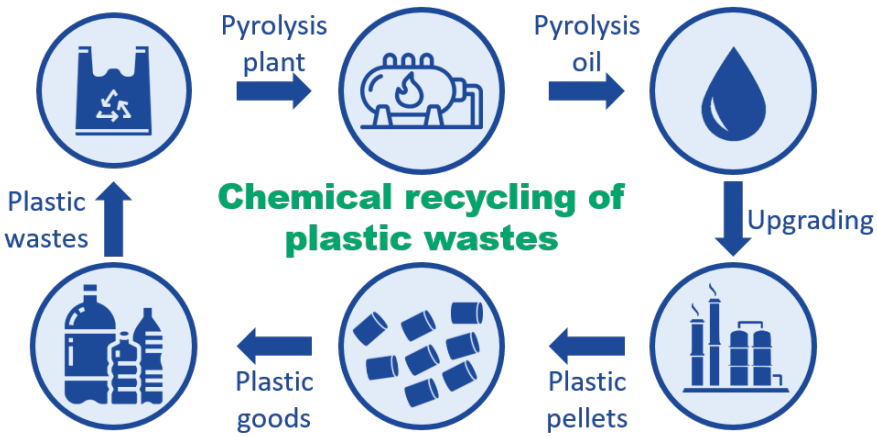

Figure 1: Chemical recycling of plastics via pyrolysis (icons taken from "https://www.drugplastics.com/an-introduction-to-advanced-plastic-recycling/ and modified").

approaches, these simulations provide temporally and spatially resolved flow fields, offering critical insights for pyrolysis reactor design. This work presents two case studies of high-performance computing (HPC) simulations for plastic pyrolysis, accompanied by key research findings that advance process optimization.

2 Simulation methods

Plastic pyrolysis involves heating shredded plastic particles to high temperatures, causing polymer degradation into short-chain and cyclic hydrocarbons (product vapors). This process constitutes a multiphase reactive flow system. For large-scale modeling of such flows, two fundamental approaches exist: The Euler-Euler approach treats both gas and solid phases as interpenetrating continua, with phase interactions (mass, momentum, and energy exchange) modeled using the kinetic theory of granular flow (KTGF) [3, 4]. While computationally efficient—solving two sets of Eulerian equations—it lacks resolution of individual particle dynamics and ignores particle size effects, which may significantly impact pyrolysis accuracy.

The Euler-Lagrange method [5] adopts a fundamentally different approach: the gas phase remains continuous, while the solid phase is treated as discrete Lagrangian parcels (LPs). Each LP represents a group of spherical particles sharing identical diameter and velocity characteristics. These parcels are tracked throughout the computational domain, with bidirectional coupling between phases achieved through source terms accounting for interphase mass, momentum, and heat transfer. Key advantages over the Euler-Euler approach include: Explicit resolution of individual particle trajectories and velocities; Incorporation of particle size distribution effects; Higher physical fidelity in multiphase interactions. However, this enhanced accuracy comes at substantially greater computational cost, making the method less practical for certain large-scale applications where Euler-Euler's approximations may suffice.

3 Results and discussions

3.1 Case I: Particle-resolved simulation

The Euler-Lagrange method assumes Lagrangian particles to be perfectly spherical and homogeneous. However, real shredded plastic particles typically exhibit irregular shapes, and the homogeneity assumption only holds for small or thermally-thin particles. Additionally, the method requires particles to be significantly smaller than the computational grid cells, preventing resolution of thermal and flow boundary layers around particles. To evaluate these limitations, we employed the Euler-Euler approach to simulate pyrolysis of a single high-density polyethylene (HDPE) particle in hot nitrogen flow. This alternative methodology enables direct resolution of both the particle-internal and its surrounding boundary layers.

As depicted in Figure 2, the simulation configuration [6] (left) and meshed computational domain (right) feature a vertical cylindrical reactor (base dimensions: diameter x length = 5.3 mm × 15 mm) with 0.35 mm quasi-equidistant grid resolution. Simulations encompassed particle diameters (2-6 mm) and geometries (sphere/cylinder/shell) across temperature regimes, with domain diameters proportionally scaled (5.3, 10.6, 21.2 mm) to maintain adequate clearance for 3, 4, 6 mm particles respectively.

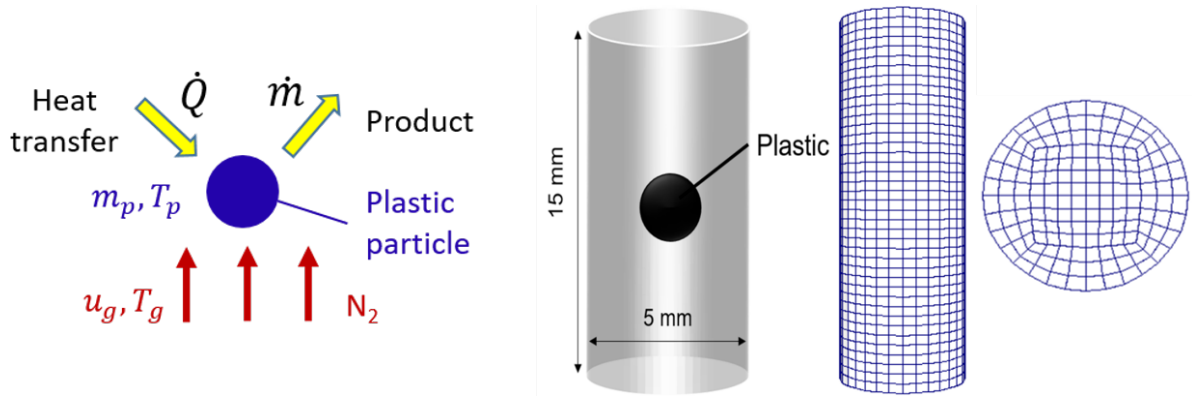

Figure 2: Setup and computational grid used for the particle-resolved simulation of plastic pyrolysis.

Figure 3 (left) displays the pyrolysis progress X (where $X = 0$ and $X = 1$ represent unpyrolyzed and fully pyrolyzed states, respectively) for plastic particles of varying diameters d_P. The results demonstrate a significant increase in pyrolysis time with d_P, attributable to greater particle mass and slower heating rates. For comparison, dotted lines show Euler-Lagrange simulations assuming ideal spherical, homogeneous particles under identical conditions. As particle size increases, particle-internal heat transfer effects become more pronounced, amplifying discrepancies between the Euler-Euler (solid lines) and Euler-Lagrange (dotted lines) methods. This is particularly evident for the 6 mm particle case in Fig. 3: the Euler-Lagrange simulation shows delayed reaction onset ($X > 0$) due to the time required to achieve uniform particle temperature – a limitation not present in the particle-resolved Euler-Euler approach, where pyrolysis initiates immediately at the hotter particle surface. The divergence between methods grows with d_P, as the Euler-Euler method better captures the thermal gradient-driven surface-initiated pyrolysis that dominates real particle behavior.

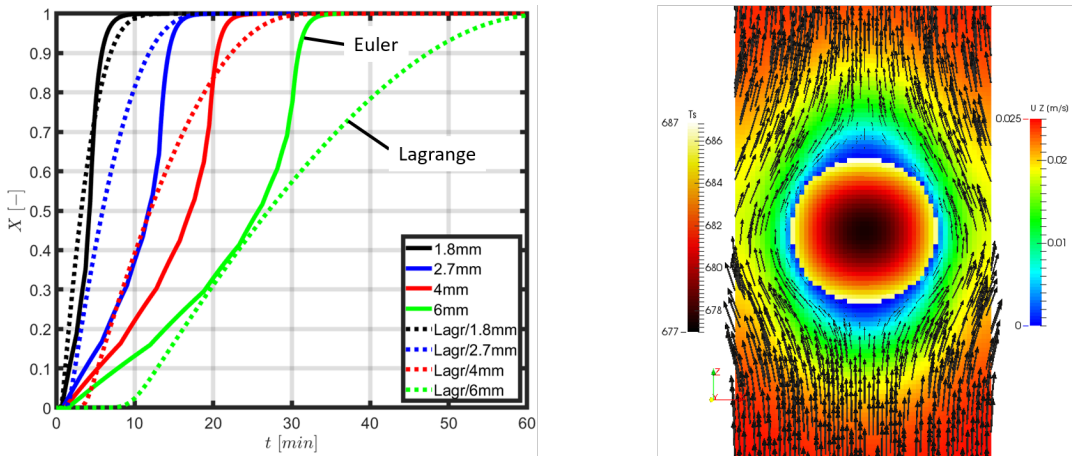

Figure 3: Time evolution of calculated conversion progress from Euler-Euler/-Lagrange approaches (left) and contours of particle temperature along with velocity vectors (right).

Figure 3 (right) presents instantaneous contours of particle temperature (T_P) and gas velocity on a meridional plane through the symmetry axis for the 6 mm particle case, with flow directions indicated by arrows. The visualization clearly reveals significant temperature gradients within the particle that are unresolvable by

the Euler-Lagrange approach, as well as boundary layer formation, where gas velocity approaches zero (no-slip condition) and temperature converges to T_P at the gas-solid interface. These findings demonstrate that the Euler-Lagrange method becomes unreliable for plastic particles exceeding 2 mm in diameter. Additional studies (not shown) further indicate substantial influences of particle shape and flow orientation on pyrolysis dynamics [7].

The simulations employed a computational grid of approximately 400,000 cells and simulated physical times up to 40 minutes. For the most computationally demanding case (6 mm particle requiring full conversion from $X = 0$ to $X = 1$), the calculations required 3 days of runtime utilizing 320 CPU cores on the bwUniCluster system at SCC/KIT.

3.2 Case II: Simulation of fluidized beds

Fluidized bed reactors offer significant advantages for plastic pyrolysis, including enhanced heat transfer, uniform temperature distribution, and continuous operation capability, making them particularly suitable for industrial-scale applications. In this study, we employ the Euler-Lagrange method to simulate a laboratory-scale fluidized bed reactor (developed at ITC/KIT) under isothermal conditions, using inert sand particles as the bed material and air as the fluidizing gas. The primary objective is to investigate the hydrodynamic behavior of the fluidized bed, focusing on particle fluidization, circulation and bubble formation dynamics, which critically influence reactor performance, such as the heat transfer.

The computational domain consists of a cylindrical reactor (60 cm length $\times$ 5 cm diameter) discretized with approximately 300,000 computational cells, yielding an average resolution of 1 mm. We examine various operating conditions by varying with bed inventory $m_S = 195 - 586$ g, superficial gas velocity $u_G = 14 - 30$ cm/s. The number of Lagrangian parcels (LPs) scales with bed inventory, reaching up to 6 million for the maximum m_S case (586 g).

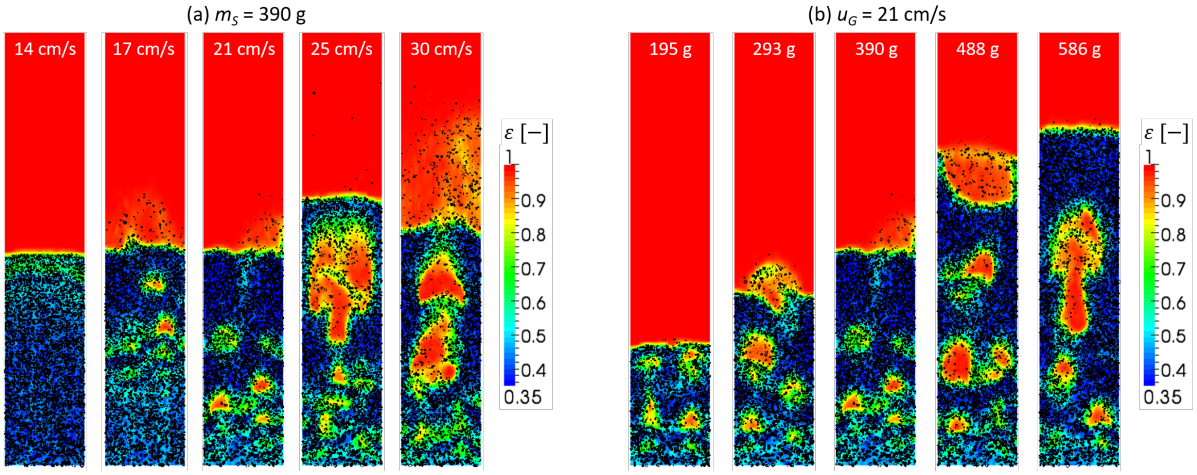

Figure 4: Snapshots of void fraction on a cutting plane passing through the centerline axis at increasing superficial gas flow velocity (a) and at increasing bed inventory (b).

Figure 4 depicts instantaneous contours of the void fraction ε (volume fraction of the gas phase) on a meridian cutting plane passing through the centerline axis for varied u_G at $m_S = 390$ g (left) and varied m_S at $u_G = 21$ cm/s (right). The solid points indicate the sand particles and the red zones surrounded by the sand particles denote the gas bubbles. The fluidization behavior observed in the experiment has been reproduced well, where an increased bubble size with u_G and an increased bed height with m_S can be detected. Although not shown here, the calculated pressure drop and bed height have shown a quantitatively good agreement with measured data, which validates the applicability of the simulations [8].

Figure 5(a) shows iso-contour of $\varepsilon = 0.66$ calculated from Euler-Lagrange simulations of fluidized beds with different reactor diameters d_R, which illustrate 3D structures of the bubbles. For the case with $d_R = 3$ cm, the hydrodynamics of the fluidized bed is dominated by large-scale bubbles with a size similar to the reactor

diameter. The formation of bubbles is significantly enhanced while up-scaling the fluidized bed, which is attributed to the increased volume for solid circulation. The same behavior with an enhanced bubble formation at larger d_R can also be detected in Fig.5(b) by the 2D contours of ε on a meridian cutting plane across the centerline axis. The results indicate an influence of up-scaling on the hydrodynamics of fluidized bed, which has a significant impact on the heat- and mass transfer behavior. This should be accounted for while designing industrial-scale pyrolysis plants using the fluidized bed technology. The reader is referred to [8] for a more detailed description of the results.

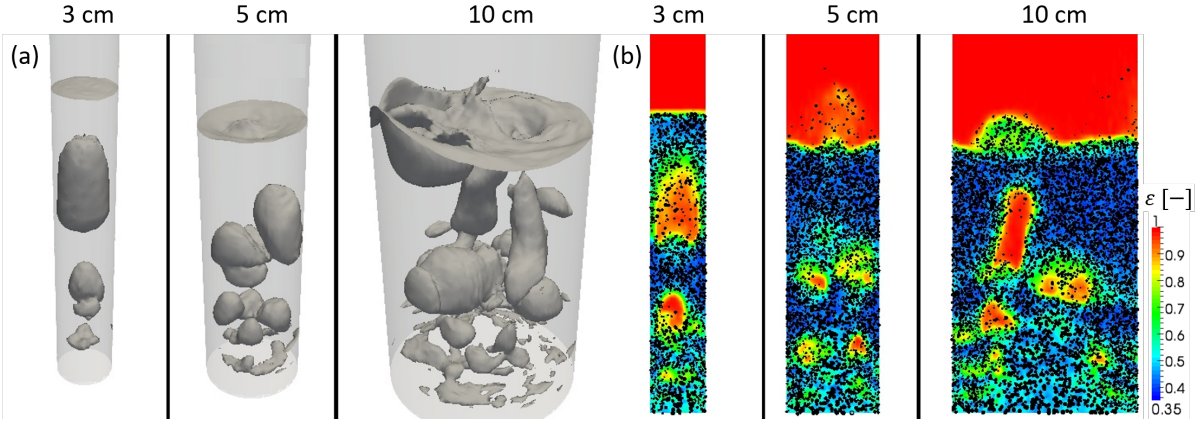

Figure 5: 3D bubble structures (a) and contours of void fraction ε on a cutting plane passing through the centerline axis (b) calculated with reactor diameters of $d_R = 3$, 5 and 10 cm.

3.3 Parallel performance

The open-source CFD software OpenFOAM has be used in this work for the particle-resolved simulations in Sec.3.1 and the simulations of the fluidized beds in Sec.3.2. It uses domain decomposition to allocate the total computational cells onto a number of sub-domains or processes, along with the message passing interface (MPI) for inter-process communication. Figure 6 on the left shows the parallel scalability and on the right the speed-up efficiency for the multiphase flow simulations (Euler-Lagrange) of the fluidized bed with $d_R = 10$ cm by using $32{\times}10^6$ and $16{\times}10^6$ LPs on the Horeka cluster at SCC/KIT, where each node has 76 CPU cores. The resolution used for the Eulerian/gas phase is 1 mm in both cases, leading to 0.56 million grid cells. The wall clock time per time step is 3.0 s for the case with $32{\times}10^6$ LPs and is 1.9 s for the case with $16{\times}10^6$ LPs, indicating that the computational effort of the Lagragian phase dominates over the computing time for the gaseous phase. Therefore, the parallel performance is better while using a larger number of LPs. The scale-up performance is good in case of using more than 100.000 LPs per core to achieve a speed-up efficiency larger than 0.8. A further increase of the number of CPU cores cannot efficiently accelerate the computing process. This is attributed to that fact that the Lagrangian parcels are located only in the lower half of the simulation domain, leading to an imbalance of computing load for each sub-domain or CPU core.

4 Conclusions

Euler-Euler and Euler-Lagrange simulations have been conducted to study the pyrolysis process of a single plastic particle with non-ideal shape and the hydrodynamic behavior of a laboratory-scale fluidized bed designed for plastic pyrolysis. The particle morphology (size, shape) has been found to play a vital role in the pyrolysis process, which is attributable to the modified condition of heat transfer as well as its impact on the pyrolysis reaction. In addition, the calculated particle circulation and bubble formation in the considered fluidized bed have shown a good agreement with corresponding experiments. Moreover, up-scaling of the fluidized beds has led to a transition from single- to multiple-column bubbling and internal particle circulation, indicating the strong influence of scale-up on the mixing and heat transfer process. In terms of an efficient utilization of HPC

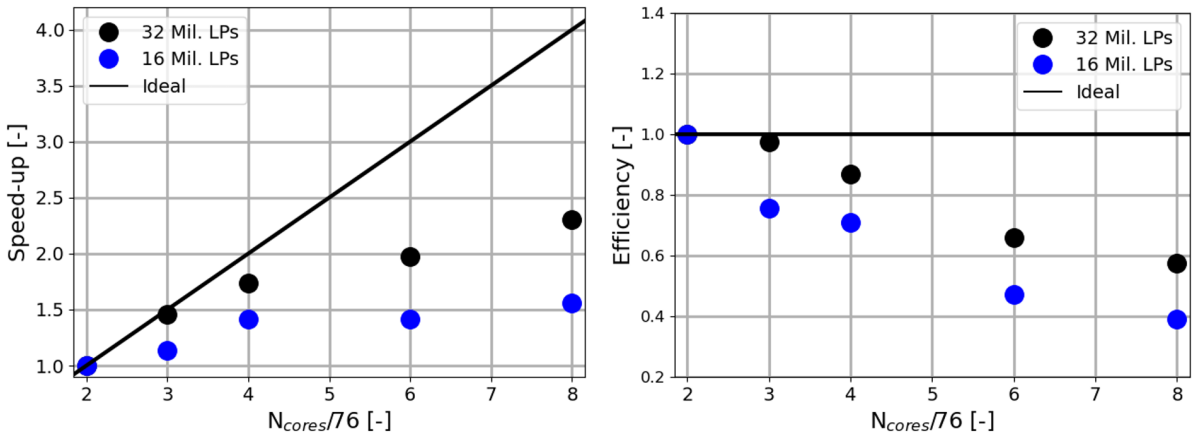

Figure 6: Speed-up performance (left) and efficiency (right) while running multiphase flow simulations (Euler-Lagrange) of fluidized beds by using 32 mil. 16 mil. Lagrange parcels (LPs) on the Horeka cluster at SCC.

resources, the usage of more than 100,000 Lagrange parcels are found to be beneficial for calculating the gas-solid flow in the current fluidized bed setup with the Euler-Lagrange method. The results reveal opportunities and challenges of numerical modeling for advancing the design process of plastic pyrolysis technology.

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