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CompArt: Next-Generation *Comp*artmental Models for Complex Systems Powered by *Art*ificial Intelligence

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ABSTRACT

Compartmental models are widely used to simplify the analysis of complex fluid dynamics systems, yet subjective compartment definitions and computational constraints often limit their applicability. The CompArt algorithm introduces an AI-driven framework that automates compartmentalization in Computational Fluid Dynamics (CFD) simulations, optimizing both accuracy and efficiency. By leveraging unsupervised clustering techniques such as Agglomerative Clustering, CompArt identifies coherent flow regions based on velocity and turbulent kinetic energy dissipation rate, ensuring a data-driven, physically consistent segmentation. The methodology integrates a connectivity-based clustering strategy, where compartments are dynamically optimized using the Silhouette score and adjacency matrix. This approach enables the reduction of high-resolution 3D CFD simulations into a network of interconnected sub-systems, significantly lowering computational costs while preserving system heterogeneity. The framework was tested on turbulent stirred tank simulations at 200 and 400 RPM, demonstrating its ability to capture both large-scale flow structures and fine-scale turbulence features. At higher RPM, increased mixing leads to a more fragmented dissipation pattern, which the model successfully adapts to. With scalability up to industrial scale meshes (~1M cells) and full automation of hyperparameter selection, CompArt enhances the applicability of CFD compartmental models in crystallization, multiphase flow, and process optimization. By bridging AI-driven clustering with physical modelling, this novel framework streamlines CFD simulations, making real-time industrial applications feasible without sacrificing predictive accuracy.

Keywords: Artificial Intelligence, Computational Fluid Dynamics, Mixing, Industry 4.0, Process Design

INTRODUCTION

Compartmental models have long been a cornerstone, offering a simplified yet effective framework for analyzing and simulating complex processes [1]. These models divide a system into interconnected compartments, each representing a sub-region with uniform properties, such as temperature, concentration, or velocity. By reducing a continuous system into discrete, manageable units, compartmental models facilitate the study of phenomena such as mass transfer, reaction kinetics, mixing dynamics and their interplay.

The strength of compartmental models lies in their ability to provide insightful approximations while significantly reducing computational demands compared to full-scale three-dimensional (3D) simulations. They are widely applied in fields such as reactive crystallization, multiphase flow, and pharmaceutical manufacturing, where understanding process heterogeneity and scaling effects is critical [2–4]. However, despite their utility, compartmental models face significant limitations that constrain their broader applicability and accuracy.

One major challenge is the reliance on expert judgment to define the number, size, and connectivity of compartments [5]. This process is often subjective, time-intensive, and prone to inconsistencies, particularly for systems with high spatial complexity. Additionally, traditional compartmental models struggle to preserve fine-scale heterogeneity, leading to oversimplified representations that may overlook critical interactions within the system.

Another limitation lies in their adaptability. Classical approaches are often tailored to specific scenarios,

requiring extensive reconfiguration when applied to new processes or scales. This lack of flexibility reduces their utility in dynamic, industrial contexts where process conditions and requirements frequently change.

Finally, the integration of multiple governing variables, such as velocity, turbulent energy dissipation rate, and temperature, remains a challenge. While these factors are crucial for accurately describing complex systems, incorporating them into compartmental models without introducing prohibitive computational costs is a significant hurdle [6].

Addressing these limitations is crucial to enhance the predictive power, scalability, and versatility of compartmental models, ensuring they remain a relevant and powerful tool in modern chemical engineering applications.

CompArt algorithm

CompArt is an innovative approach to modelling complex systems, based on Computational Fluid Dynamics (CFD) simulations. CFD plays a crucial role in various industries such as chemical engineering, pharmaceuticals, and energy, where understanding fluid flow, heat transfer, and mass transport is vital for optimizing process performance. However, simulating large-scale 3D systems is computationally expensive, which limits their real-time applicability in industrial applications. The CompArt project addresses this challenge by exploiting artificial intelligence (AI) to reduce computational costs without compromising the fidelity of the simulation results.

Objectives

The primary goal of the CompArt project is to innovate the way complex systems are modelled. A central ambition of the project is the integration of unsupervised AI-driven clustering techniques to automate the compartmentalization process. Traditionally, determining the optimal number of compartments for a CFD simulation has relied heavily on expert knowledge, requiring iterative manual adjustments to balance computational cost and simulation accuracy [7]. By using AI, CompArt automates this process, enabling the system to autonomously define the most suitable number of compartments based on input parameters. This not only reduces the dependence on domain-specific expertise but also enhances the consistency and efficiency of the modelling process.

Scalability is another cornerstone of the project. By representing the 3D system as a network of interconnected sub-systems, CompArt provides a structured way to reduce the computational burden associated with CFD simulations. Each compartment is characterized by uniform properties, such as velocity or turbulence dissipation rates, which significantly simplifies the mathematical complexity of the problem. This reduction allows for real-time simulations, even in industrial contexts where rapid decision-making is essential.

Finally, CompArt places a strong focus on preserving the heterogeneity and spatial characteristics of the system. While simplifying the model, the framework ensures that the inherent complexity of the system, such as variations in flow dynamics or reactive processes, is not lost. This attention to detail is particularly critical in applications like crystallization, where system heterogeneity plays a vital role in determining the outcome of processes. By maintaining these features, CompArt strikes a balance between computational efficiency and the fidelity required for accurate simulations.

METHODOLOGY

Simulation Setup and Governing Equations

To test the proposed methodology, simulations are performed on 3D stirred tanks. The simulations use the Reynolds-Averaged Navier-Stokes (RAS) approach with the $k-\varepsilon$ turbulence model. The governing equations include the incompressible Navier-Stokes equations, along with transport equations for turbulent kinetic energy (k) and its dissipation rate (ε)

$$\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u}\cdot\nabla\boldsymbol{u} = \nu_t\nabla^2\boldsymbol{u} - \frac{1}{\rho}\nabla p + \boldsymbol{g} \quad (1)$$

$$\frac{\partial k}{\partial t} + \boldsymbol{u}\cdot\nabla k = \Gamma_{t,k}\nabla^2 k + \frac{P}{\rho} - \varepsilon \quad (2)$$

$$\frac{\partial \varepsilon}{\partial t} + \boldsymbol{u}\cdot\nabla\varepsilon = \Gamma_{t,\varepsilon}\nabla^2\varepsilon + \frac{C_{\varepsilon 1}\varepsilon}{k}\frac{P}{\rho} - \frac{C_{\varepsilon 2}\varepsilon^2}{k} \quad (3)$$

$$\nu_t = \frac{C_\mu k^2}{\varepsilon} \quad (4)$$

The Navier-Stokes equations describe the motion of an incompressible, Newtonian fluid, where turbulence effects are modeled through the turbulent viscosity (ν_t). This additional viscosity accounts for the enhanced momentum diffusion due to turbulent eddies, which cannot be directly resolved in a Reynolds-Averaged Navier-Stokes (RAS) framework.

The turbulent kinetic energy equation (k) quantifies the energy associated with turbulent velocity fluctuations. It includes terms for production (P), which arises from the mean velocity gradients, dissipation (ε), which represents the conversion of turbulent energy into thermal energy, and diffusion (Γ_t) to account for spatial transport of turbulence.

The turbulent dissipation rate equation (ε) governs the rate at which turbulent kinetic energy is dissipated into smaller scales.

AI-driven Clustering for Compartmentalization

Clustering plays a pivotal role in compartmentalization by grouping cells in the mesh based on similar characteristics. Several clustering methods were considered,

including k-means and DBSCAN. However, we focused on using Agglomerative Clustering, which is an unsupervised neural network that maps high-dimensional data onto a lower-dimensional (embedded) space, preserving the topological relationships in the input data. This algorithm is well-suited for clustering spatial data in CFD simulations, as it can efficiently handle the inherent complexity of fluid dynamics and capture system heterogeneity.

The AI-driven model autonomously determines the optimal number of clusters based on the user-defined input parameters, such as velocity and turbulent kinetic energy dissipation rate, using the Silhouette score as a quantitative metric. The Silhouette score evaluates the quality of clustering by measuring how similar a data point is to its cluster compared to other clusters, indicating the cohesion and separation of the clusters.

Feature Processing and Connectivity

In CFD simulations, the fluid domain is represented as a mesh of interconnected cells, and dividing this mesh into meaningful compartments requires a robust understanding of cell connectivity. To achieve this, a connectivity matrix is constructed to capture the relationships between neighboring cells efficiently. Leveraging parallel computation, the matrix is built using a sparse format, significantly reducing the computational time and making the process suitable for large-scale meshes. Once the connectivity is established, the input features, such as velocity and turbulent dissipation rate, are normalized. This normalization, performed using standard scaling techniques, prepares the data for effective clustering. To enhance the accuracy of the Agglomerative Clustering algorithm, key hyperparameters are optimized using the Silhouette score, automating the process and eliminating the need for expert-driven adjustments. This streamlined approach ensures efficient and reliable compartmentalization of complex systems, paving the way for broader application in industrial simulations.

RESULTS

The results underscore the effectiveness of unsupervised algorithms in clustering CFD data, accurately identifying zones with differing velocities, as shown in Figure 1. However, velocity alone is insufficient to capture the complexity of processes like reactive crystallization [8], where the turbulent kinetic energy dissipation rate plays a crucial role in flow dynamics and system behavior. By incorporating both velocity and turbulence dissipation as input features, the clustering algorithm produces a more refined segmentation, effectively capturing system heterogeneity.

The velocity and turbulence dissipation rate fields at 200 and 400 RPM, shown in Figure 1, were processed using the CompArt algorithm to generate dynamically optimized compartments. The compartmentalization strategy was guided by two key criteria: the silhouette metric, ensuring well-defined clusters, and cell connectivity, preserving the physical consistency of adjacent regions. The resulting segmentation effectively captures both large-scale flow structures and fine-scale turbulence features. At 200 RPM, turbulence dissipation is more localized near the bottom and walls, whereas at 400 RPM, the enhanced mixing leads to a greater number of high-dissipation regions.

A crucial observation is the ability of the algorithm to adapt to changes in the flow and turbulence fields as the RPM increases. At 200 RPM, the region with the highest variation in velocity and turbulence is concentrated near the impeller. However, as the rotational speed increases, the system becomes globally more turbulent, leading to the formation of strong gradients, particularly in stagnant zones (below the impeller) and at the interface between the bulk fluid and the wall (wall effect). Even for an expert, it would be challenging to manually delineate these zones accurately, whereas CompArt successfully identifies them. A particularly evident example is the stagnant fluid region below the impeller. In crystallization processes, this reactor zone can lead to Critical Quality Attributes (CQA) of the product that do not meet specifications, as particles in this region can grow or agglomerate due to prolonged residence times.

Another notable feature of CompArt is its ability to define clusters composed of just a few layers of cells. In both cases, a distinct compartment is observed wrapping around the impeller shaft. It is important to note that, although at lower magnitudes, the shaft also rotates at a certain velocity, thereby exchanging momentum with the surrounding fluid. This characteristic is captured by the algorithm, enabling the monitoring of processes such as secondary nucleation or agglomeration, which are directly linked to turbulent kinetic energy dissipation near moving walls.

These findings highlight the robustness of the CompArt framework in systematically identifying meaningful compartments while preserving spatial heterogeneity and flow physics. By integrating data-driven clustering with physical constraints, this methodology provides an efficient and adaptive approach for reducing CFD complexity while maintaining predictive accuracy.

CONCLUSIONS

The CompArt framework demonstrates a significant advancement in the compartmental modelling of fluid dynamics systems by integrating AI-driven clustering techniques with CFD simulations. Through the application of Agglomerative Clustering, the methodology effectively partitions the computational domain into meaningful

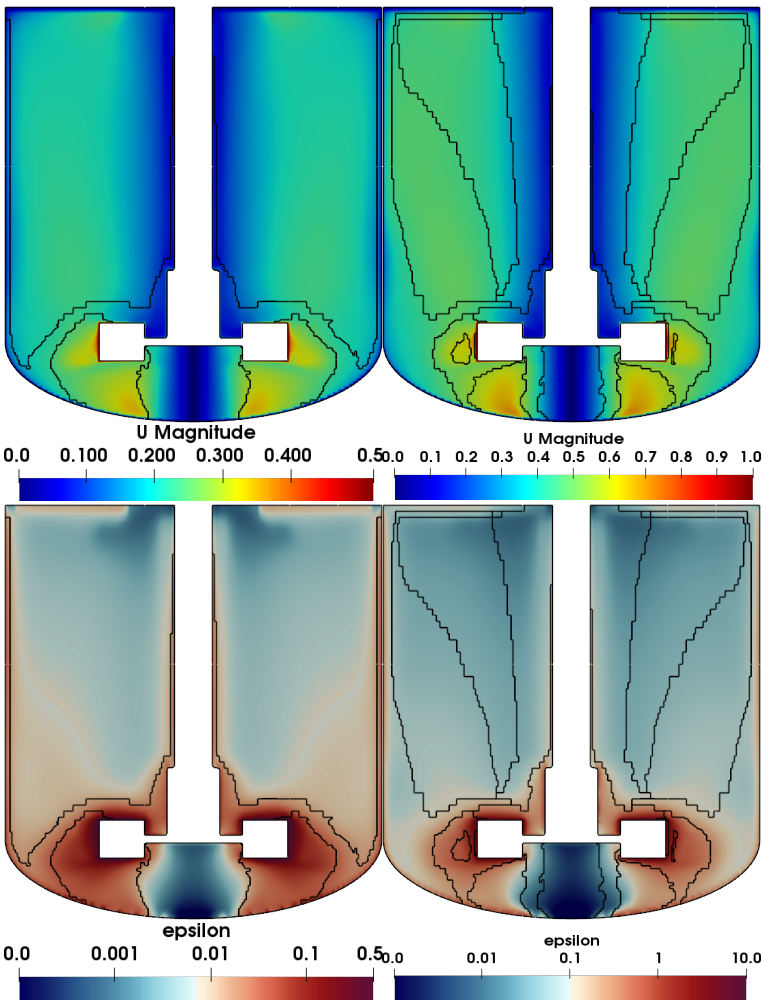

Figure 1: Velocity (*top row*) and turbulence dissipation rate (*bottom row*) compartmentalized fields at 200 RPM (*left*) and 400 RPM (*right*). The compartmentalization was performed using the CompArt algorithm.

compartments, preserving the spatial heterogeneity and critical flow structures. This novel approach addresses the key limitations of traditional compartmental models by eliminating the reliance on expert-driven segmentation and enhancing the adaptability of the model across different process conditions.

One of the primary strengths of CompArt is its ability to autonomously determine the optimal number of compartments based on quantitative metrics such as the Silhouette score, ensuring well-defined and physically relevant clusters. Additionally, the framework's capacity to incorporate multiple variables, such as velocity fields and turbulent kinetic energy dissipation rates, allows for a more accurate representation of flow dynamics, which is crucial in applications like crystallization and multiphase flow systems.

The studies at different rotational speeds (200 and 400 RPM) illustrate the robustness of the approach. The model successfully captures key flow features, such as the formation of strong turbulence gradients near stagnation zones and wall regions, which are critical in industrial applications. The ability of the algorithm to detect small-scale but significant structures, such as the interaction of the impeller shaft with the surrounding fluid, further underscores its capability to enhance predictive accuracy.

By reducing computational complexity while maintaining fidelity, the CompArt framework provides a scalable and efficient tool for industrial CFD simulations. Its automation, adaptability, and accuracy make it a promising solution for optimizing process performance in various engineering domains, facilitating real-time decision-making and improved process control.

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