

From Three-Body Problems to Mesoscale Intelligence: A CFD-Based Deep Reinforcement Learning Intelligent Control Method

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Abstract

This study defines the “three-particle system” for the first time as the minimum complex unit at the mesoscale connecting microscopic mechanisms and macroscopic behavior in multiphase flows. Drawing on the concepts of chaos and competition from the “three-body problem,” it reveals the essential contradictions between synergy-antagonism, and local non-uniformity versus global uniformity, occurring during the droplet coating process of three particles. On this basis, an intelligent closed-loop control framework was constructed by coupling a Computational Fluid Dynamics (CFD) Volume of Fluid (VOF) model with a Distributed Soft Actor-Critic (DSAC) deep reinforcement learning algorithm, achieving dynamic regulation of droplet injection velocity and radius. The agent perceives the liquid film distribution in real-time through 33 flow field probes, autonomously stabilizing the Weber number within the optimal range (115), and discovers a counter-intuitive control law: rather than pursuing absolute uniformity at every control step, it achieves statistical global uniformity at the cost of local mesoscale non-uniformity through alternating biases in the time domain. Consequently, this paper proposes the new concept of “Mesoscale Intelligence” or “Meso-Intelligence,” emphasizing cross-scale intelligent control strategies that are based on mesoscale mechanisms, explainable, and transferable. It systematically addresses three core questions: what the mesoscale structure is, why it arises, and how it influences macroscopic behavior. This work provides a new path for the deep integration of multiphase reaction engineering and artificial intelligence, with potential application value in fields such as fine chemicals, pharmaceutical coating, and microfluidic encapsulation.

Full Text

Preamble

From Three-Body Problems to Mesoscale Intelligence: Deep Reinforcement Learning-Based Intelligent Control Methods

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In the context of multiphase reaction processes in chemical engineering, the minimum topological unit composed of three particles can be defined as the “three-body problem” of multiphase flow. We propose that this problem serves as a core mesoscale hub connecting microscopic mechanisms with macroscopic behavior. Similar to the chaos and unpredictability revealed by three-body motion in celestial mechanics, a three-particle system during the droplet coating process exhibits complex synergy and non-uniform distribution behaviors. These phenomena cannot be fully captured in two-particle systems, yet they are easily obscured by statistical averaging in many-particle systems. Therefore, systematically resolving the particle interaction mechanisms within this “minimum complex unit” is a critical breakthrough for revealing the evolution laws of mesoscale structures and achieving active intelligent control. It serves as the theoretical prerequisite for developing explainable and transferable cross-scale intelligent control strategies.

In industrial processes such as spray granulation and catalyst modification, the uniformity of droplet coating on particle surfaces directly determines product quality. However, the inherent nonlinearity and randomness of multiphase flow systems, combined with the violent evolution of gas-liquid interface topology, make achieving uniform liquid film distribution among multiple particles extremely challenging. Traditional open-loop control strategies—utilizing fixed injection velocities and droplet sizes—cannot adapt to dynamic changes in flow states, making it difficult to simultaneously balance single-particle coverage with inter-particle coating uniformity. We have constructed a closed-loop control framework coupling the Volume of Fluid (VOF) model with a Distributed Flexible Actor Deep Reinforcement Learning (DRL) algorithm, successfully achieving intelligent regulation of the droplet coating process in a three-particle system. The agent perceives liquid film distribution in real-time through flow field probes and dynamically adjusts the droplet injection velocity and radius. It autonomously discovered that by stabilizing the Weber number within an optimal range, liquid film spreading capability is maximized while avoiding droplet breakup or retraction. More importantly, this research reveals a counter-intuitive control logic regarding mesoscale variables: the agent does not pursue absolute uniformity at every individual control step. Instead, it utilizes alternating biases in the time domain, sacrificing local instantaneous unifor-

mity to achieve global statistical uniformity. This demonstrates that local non-uniformity is a necessary path toward achieving global uniformity. The CFD-DRL framework reveals the mesoscale regulation mechanisms within multiphase coating processes, proving that deep reinforcement learning can autonomously emerge physically explainable intelligent strategies from high-dimensional, unsteady flow environments. At the application level, the framework exhibits strong adaptability to both dispersed and compact particle arrangements, spontaneously switching control logic. This provides a new path for intelligent control in fine chemical processes with high uniformity requirements, such as precision drug coating and functional microsphere preparation. Furthermore, these strategies can be distilled into empirical correlations or feedforward rules to be embedded into traditional control systems. By introducing the “three-body” concept into multiphase flow mesoscale research, we define it as the minimum complex unit bridging the gap between two-body systems (which are overly simplistic) and many-body systems (where mechanisms are masked by statistical averaging). “Mesoscale Intelligence” differs from traditional “AI for Science” by emphasizing explainable, transferable control based on mesoscale mechanisms.

Taking the three-particle coating problem as an example, the DRL closed-loop control framework discovered counter-intuitive control laws: achieving global uniformity through local non-uniformity and temporal alternating biases, rather than pursuing uniformity at every step. This proposes a path for the deep integration of multiphase reaction engineering and artificial intelligence, opening new avenues for the cross-scale intelligent control of complex multiphase processes. For further research background and details, please refer to [?]. We can further expand our thinking: based on the study of the droplet coating process in three-particle systems, we refer to the series of intelligent autonomous regulation mechanisms discovered in the three-body liquid film system as “Mesoscale Intelligence” (or more broadly, “Meso-Intelligence”). While traditional research simply uses AI methods to empower or assist in material R&D and process optimization to shorten trial-and-error cycles without distinguishing between scales and levels, Meso-Intelligence focuses on the mesoscale mechanisms situated between the macro-process and the underlying micro-scale information (atoms, molecules, or particles). It attempts to discover whether universal mesoscale structures or mechanisms exist across different processes, aiming to answer three questions: What are the mesoscale structures in different systems? Why do these mesoscale structures arise? What are the control mechanisms behind these structures, and what impact do these mesoscale mechanisms/structures have?

Taking chemical process intensification as an example, research into Meso-Intelligence reveals the complex mesoscale mechanisms and implementation pathways of process intensification.

参考文献

Guan, Yang, Chem.

Note: Figure translations are in progress. See original paper for figures.

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