Chapter 2
The EMMS Principle: Compromise Between Competing Dominant Mechanisms

2.1 The Importance of Structural Heterogeneity

Dynamic heterogeneous structures that appear on the mesoscales between element and system scales make correlating microscale and macroscale difficult (Fig. 2.1). Such heterogeneous structures are currently bottlenecks that prevent us from fully understanding the behavior of complex systems in science, engineering, nature, and even society.

The universe contains heterogeneous structures that form on different levels through complex dynamic processes. According to the Standard Model of particle physics [51], elementary particles of matter are quarks and leptons (including electrons), and gauge bosons act as force carriers. Two quarks form a meson, and three quarks form a baryon (including nucleons). Therefore, mesons or baryons are structures at the lowest level known to date. Fewer than 300 nucleons form an atomic nucleus, which is the level of structure above nucleons. Atomic nuclei and electrons can form plasma, or an atomic nucleus and fewer than 120 electrons can form an atom, which are another level of structures. Atoms form molecules, macroscopic gases, or condensed matter, representing structures at even higher levels. Huge amounts of condensed matter form planets, whereas very large amounts of gases or plasma form stars. Planets form a planetary system around a star, and stars with planets form galaxies [52], which can further form groups, clusters, and even superclusters [53]. Superclusters are currently the highest level structures in the observable universe. We consider that heterogeneity (cf. Fig. 6.3) exists in most systems [7].

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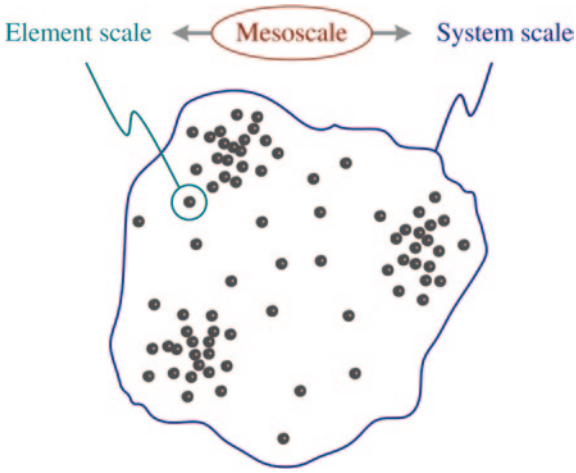

Fig. 2.1 Mesoscale between a single element and system

Chemistry, materials science, and condensed matter physics focus on the dependence of bulk material properties on atomic or electronic structures [54]. The structures of molecular clusters have become another focus in recent years with the development of supramolecular chemistry and nanotechnology [55]. These fields include not only the stationary structures at equilibrium state but also the dynamic processes prevailing during their formation. Geology [56] and astronomy [57] investigate the inner and outer structures of the earth and celestial objects. Meanwhile, biology [58] studies the structures of organic molecules, cells, tissues, organs, and their interdependence. Biology also probes further downwards to genes and upwards to systems.

Chemical engineering often involves dynamic structures. Dynamic structures are mostly complex, making it difficult to scale-up reactors. Without appropriate understanding of dynamic structures, quantitative design and control of processes is seldom possible. However, insufficient attention has been paid to understanding dynamic structures because no unifying theory governing all complex systems exists, and complexity science itself is still a field of "perplexity" [59]. Therefore, dynamic structures are a challenge not only for chemical engineering but also for all other fields investigating complex systems. Chemical reactors can be designed and optimized quantitatively only when various structural changes in systems can be predicted.

We initially studied particle clustering in gas–solid two-phase flows. Such particle clustering is a typical mesoscale phenomenon, featuring the interaction at or between three scales: the microscale of individual particles, mesoscale of particle clusters, and macroscale of the global system [5, 6], which was the starting point of this series of research.

The three cases of structures shown in Fig. 2.2 have the same element (particle), system volume, and number of particles. However, they have quite different mesoscale structures, which lead to different transport and reaction performance.

Both local structure and overall structure in gas–solid systems affect system properties. Figure 2.2 shows the considerable difference of transfer rate, represented here by the drag coefficient C_D, for different structures with the same amount of solid particles in a given volume (i.e., the same average voidage) and the same gas flow rate [15]. Local structure leads to a decrease in C_D from Fig. 2.2(a) to (b), even though the average parameters for these two structures are identical. Overall structure leads to a further decrease of C_D from Fig. 2.2(b) to (c), indicating that the formation of a core-annulus structure reduces the global transfer rate. The contribution of dynamic changes in a structure to mass transfer rate has been further demonstrated experimentally [25, 35]. Therefore, it is important to understand these structural changes and their influence on transport phenomena during predicting the performance of chemical reactors, which is the most challenging issue in chemical engineering.

2.2 Analysis of Heterogeneous Structures

Heterogeneous structures are common in all multiscale systems. They may be analyzed by one of the following three approaches:

- The first is the ***discrete method***, which is based on known information at the element scale, and tries to understand complex systems at higher scales by analyzing lower-scale mechanisms. However, if the lowest-scale mechanisms are not fully understood, any deviation at this scale is magnified at higher scales. In addition, discrete

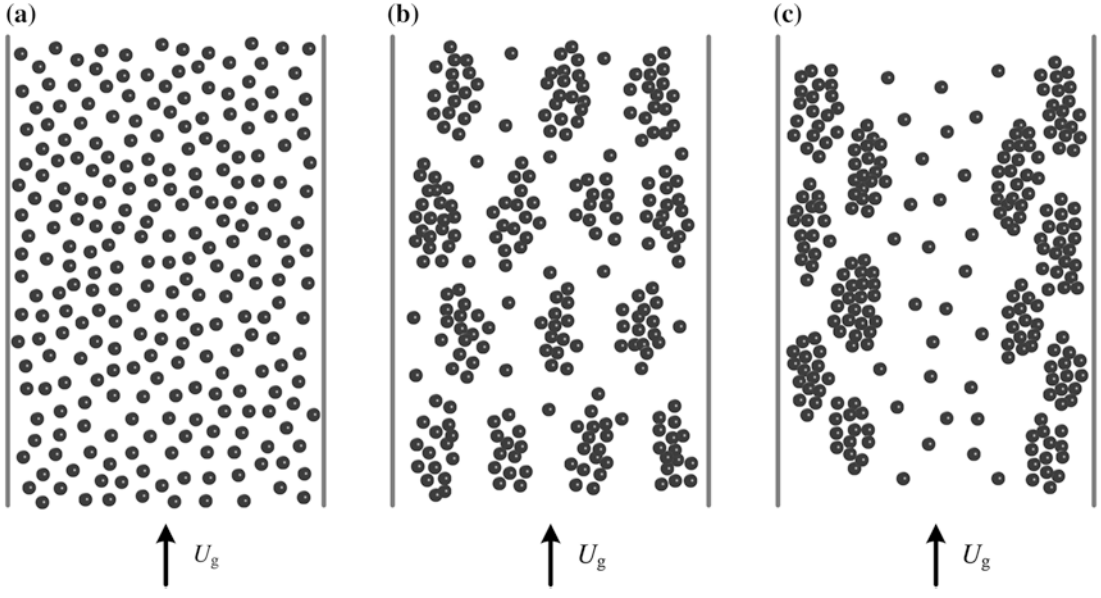

Fig. 2.2 Critical dependence of transport behavior on mesoscale structure. **a** Without structures $C_D = 18.6$. **b** With only local structures $C_D = 5.43$. **c** With both local and global structure $C_D = 2.85$. Reprinted from [15], Copyright 2013, with permission from Elsevier

approaches have high computation cost, so it remains difficult to simulate large systems.

- The second is ***averaging*** all parameters over specific space or time by considering the system to be spatially or temporally uniform. This is the simplest approach and is usually practical. However, it cannot correctly describe heterogeneous structures, leading to errors.
- The third approach involves taking the ***multiscale*** structure into account and considering the disparity of behaviors and interactions at and/or between different scales.

Among these three approaches, the averaging one, although commonly used, is not sufficient to formulate transport phenomena in heterogeneous structures because it does not distinguish between different scales. This is shown in Fig. 2.3 for gas–solid two-phase systems consisting of a solid-rich dense phase and gas-rich dilute phase. Gas–solid interaction displays a multiscale nature involving three different mechanisms [19, 21, 28]:

- ***"Particle-dominated"*** in the dense phase, that is, particle movement is realized by suppressing gas movement.
- ***"Gas-dominated"*** in the dilute phase, which means that the gas movement is realized by suppressing particle movement.
- ***"Particle-gas-compromising"*** between the dilute and dense phases. Here, the movement of neither the gas nor the particles dominates, and therefore, they compromise.

If the averaging approach is used, these three different mechanisms will be blurred, and the value of C_D will be distorted, as shown in Fig. 2.3. The data in Fig. 2.3 have been calculated for a particle-air system [19], where the particle diameter is 54 μm, the particle density is 930 kg/m^3, the solid flow rate is 50 kg/(m^2·s), and the gas velocity is in the range between 1.5 and 3.2 m/s.

In conclusion, most structures in chemical engineering are multiscale, which cannot be appropriately quantified by the averaging approach. The discrete approach based on microscale mechanisms are not yet practical because of the limitations of measurement technology and computer capacity. Multiscale methodology was, therefore, considered as a promising approach for describing both stationary and dynamic structures. However, a generalized methodology had not yet been developed, which stimulated this series of study at IPE, CAS in the 1980s.

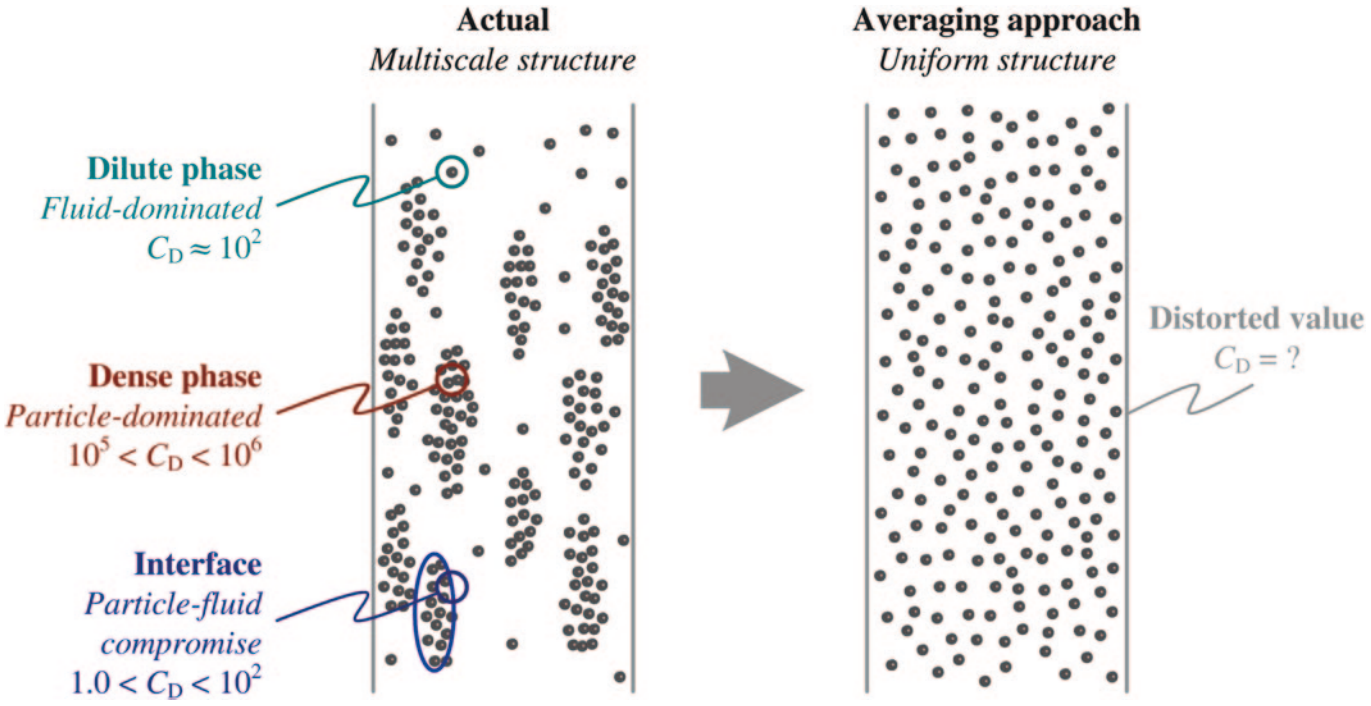

Fig. 2.3 Insufficiency of the averaging approach in analyzing multiscale structures. Reprinted from [15], Copyright 2013, with permission from Elsevier

2.3 Multiscale Approaches to Analyze Heterogeneity

Multiscale methods are commonly used in different fields, although most do not use the term 'multiscale.' In fact, both scientists and engineers frequently consider multiscale problems, either intentionally or unintentionally. Multiscale methods can be roughly divided into three types [7, 15]: descriptive, correlative, and variational, as shown in Fig. 2.4.

The most popular is the ***descriptive*** multiscale method, which is widely used to identify various structures at different scales without, however, accounting for their mechanism of formation, e.g., in image analysis, material characterization, numerical computation, and morphology. Although this method is used mainly for stationary structures, dynamic structures can also be described when statistical properties of structures are needed. Mathematical tools such as wavelet analysis [31] have been used for this purpose.

The ***correlative*** method tries to establish the relationship between parameters at different scales. This bridges the parameters at element scale with those at system scale by applying coarse graining, constitutive equations, and statistical mechanics. However, it is difficult to establish such a bridge, and the governing rule of the relationship between different scales has not been physically revealed. Accordingly, different approaches are usually based on different assumptions, which can introduce errors. Although much effort has been expended in this kind of analysis, it is not well understood yet.

Most current literature on this topic is related to descriptive and correlative multiscale methodologies.

To correlate different scales that contribute to the formation of multiscale structures, the ***variational*** multiscale methodology follows a different strategy to those described above. It stipulates that (1) multiscale structure arises from the stability condition of a given system [5, 6, 19], and (2) the phenomena at different scales are determined by this stability condition. Therefore, in addition to structural resolution at each scale, stability conditions are established to reflect the correlation between scales, which involves mesoscale modeling.

Different disciplines at different levels (cf. Fig. 6.3) deal with multiscale problems in various ways, but mostly with coarse graining or

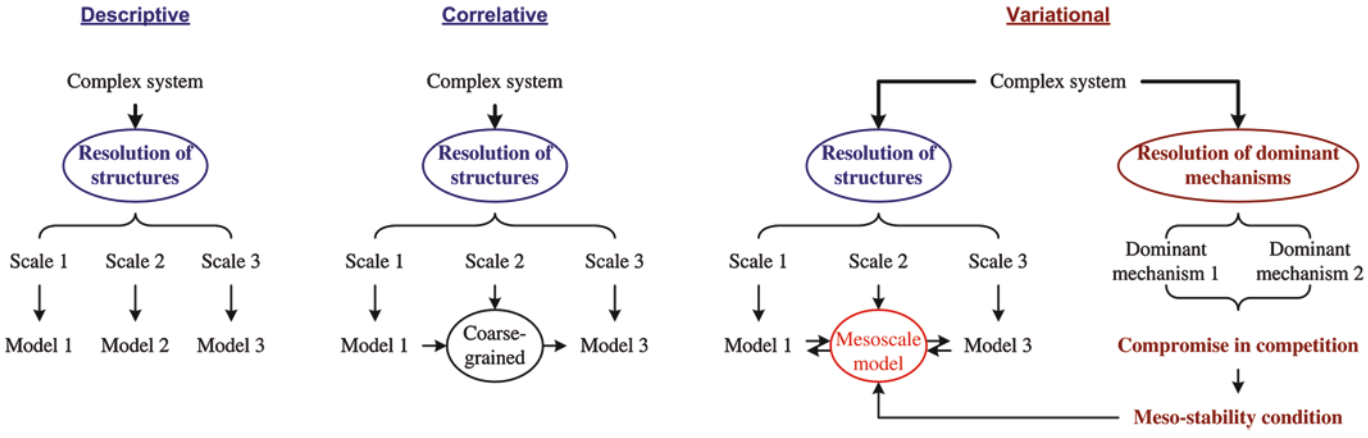

Fig. 2.4 Multiscale methodologies: descriptive, correlative, and variational

statistical approaches, that is, an averaging approach, which is because of the lack and/or ignorance of the governing principle that rules phenomena at mesoscales. Variational approaches aim to overcome this problem by identifying the stability conditions of structures at these mesoscales to correlate parameters at microscales and macroscales. In fact, a stability condition must be needed when structures are studied, without which the formation mechanism of structures cannot be revealed, and the correlation between parameters at different scales cannot be established.

The variational multiscale methodology also recognizes the multiplicity of multiscale structures, however, because it is difficult to formulate stability conditions, variational multiscale methodology has not yet been sufficiently explored, as reviewed in [7, 12].

Both the correlative and the variational methods can be of help to coarse-grained models and constitutive equations, but in different ways: The former is through graining microscale interactions, which is a unidirectional correlation, and has been applied widely; The latter is through providing with a governing rule or a stability criterion in a bidirectional correlation, deserving to be explored in the future, as discussed in this brief.

2.4 A Variational Multiscale Method: The EMMS Model

It is obvious that correlative and variational methods are devoted to establishing mesoscale models but from different angles: the variational method uses a stability condition and the correlative one grains element behaviors. The EMMS model [15] is a variational method that originated from the analysis of particle clustering in gas–solid fluidization, and is a typical mesoscale model. As illustrated in Fig. 2.5, a gas–solid fluidization system contains a heterogeneous structure, roughly consisting of dense and dilute phases, with an average voidage ε at the global scale under the operating conditions U_g and U_p. At the particle scale, individual particles interact with the gas with different parameters in the dense and dilute phases (here, we assumed uniformity in both dense and dilute phases). At the mesoscale between the particle and global scales,

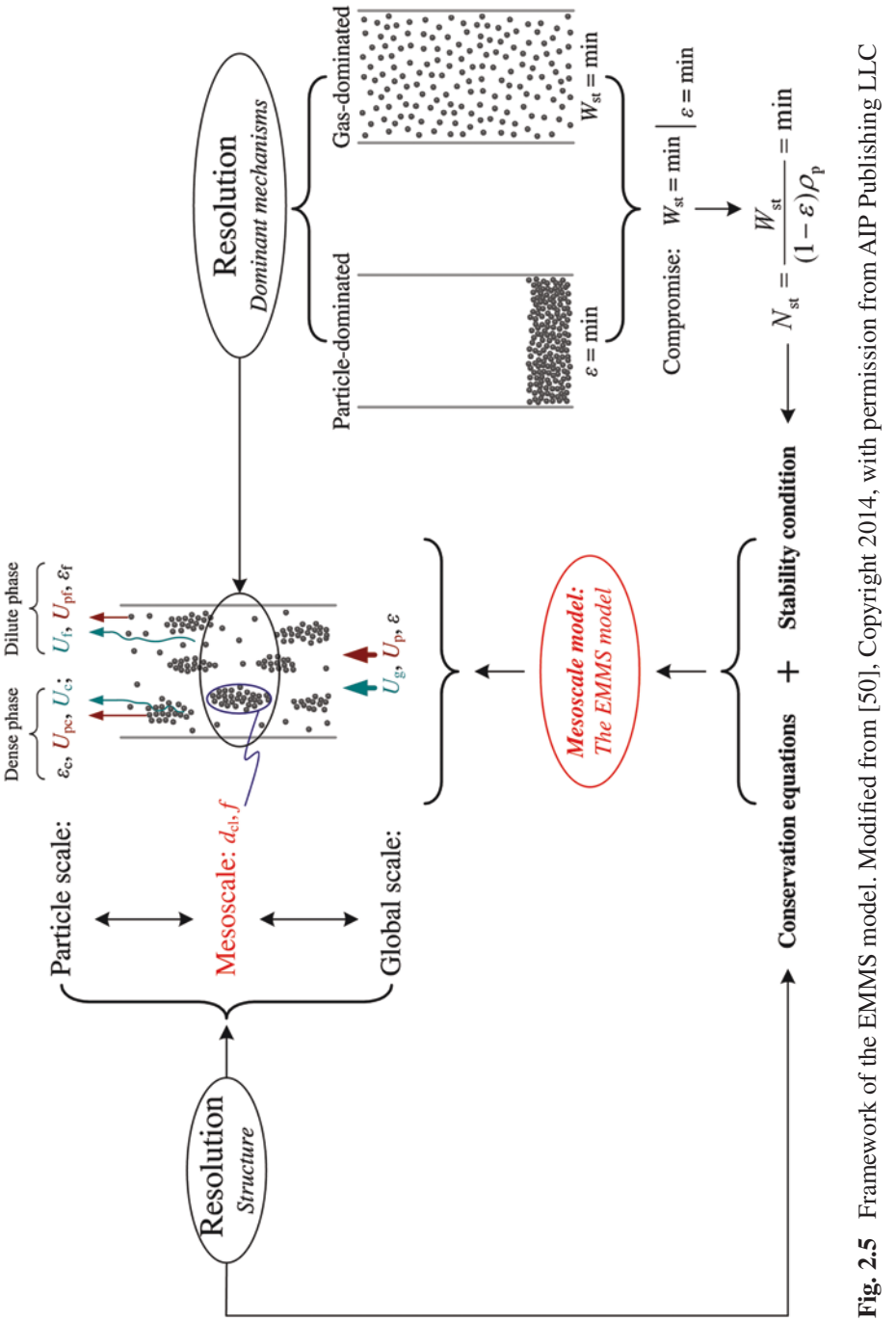

Fig. 2.5 Framework of the EMMS model. Modified from [50], Copyright 2014, with permission from AIP Publishing LLC

complicated dynamic particle clusters form; these represent the collective behavior of particles. These dynamic clusters complicate the modeling of gas–solid fluidization systems.

Correlating the global parameters U_g, U_p, and ε with the particle-scale parameters ε_f, U_{pf}, and U_f for the dilute phase and ε_c, U_c, and U_{pc} for the dense phase is a challenge. We therefore included mesoscale parameters f and d_{cl}, which call for an additional condition besides conservation equations since the number of variables is larger than the number of equations available. While looking for this additional condition, we recognized that the resolution of dominant mechanisms had to be analyzed in addition to structure resolution. The compromise between the dominant mechanism of particles, $\varepsilon = \min$, and that of the gas, $W_{st} = \min$, defines the stability condition of the system, and correlates the parameters at different scales. That is, the energy consumption for suspending and transporting particles per unit mass $N_{st} = \min$, leading to the EMMS model (Fig. 2.5).

From the EMMS model, eight parameters (ε_f, U_{pf}, U_f, ε_c, U_c, U_{pc}, f and d_{cl}) at three scales can be solved, and regime transitions with totally different transport behaviors can be defined [19]. In particular, the EMMS model can predict the phenomenon of choking, which is a jump change in structure, from operating conditions and material properties [19, 21].

This is the first version of the EMMS model [5, 6, 19]. At the beginning of this work, we used the term "coordination" and $N_{st} = \min$ to describe the compromise in competition between gas and solids because the extremum behavior of gas $W_{st} = \min$ and that of solids $\varepsilon = \min$ were not yet well understood (in Chinese, "coordination" means action of compromise in competition). After establishing the EMMS model to describe mesoscale structure, it was extended to calculate the radial distribution of heterogeneity assuming a global stability condition (the integrated average of N_{st} over the cross-section) [19, 20]. The EMMS model was able to explain why the so-called core-annulus structure forms in fluidized beds. Then, we examined the concept of "compromise in competition" further to elucidate the mechanism of choking, which occurs under critical conditions as a sudden change in structure from a dilute uniform state to a dense two-phase state [28, 29].

With the recognition of the gas movement tendency of $W_{st} = \min$ and that of solids of $\varepsilon = \min$, the concept of compromise in competition

between gas and solids was further clarified into three regimes [28, 29, 60]: gas-dominated with $W_{st} = \min$, gas–solid compromising with $W_{st} = \min|_{\varepsilon = \min}$, and solid-dominated with $\varepsilon = \min$. Thereafter, we focused on the compromise regime, defined as the "***compromise in competition between different dominant mechanisms***," that is, the compromise between $W_{st} = \min$ and $\varepsilon = \min$, which we then termed the EMMS principle. Here, an extremum represents "competition," and "coordination" implies the responding action in the compromise in competition.

In fact, the mechanism of the stability condition should be the key to solving problems involving dynamic structures. However, it was neglected as researchers looked for alternative solutions such as coarse graining, constitutive, and statistical models for describing dynamic systems.

In a subsequent study, we further confirmed the principle of compromise in competition [23]. In particular, the universality of the EMMS principle was first explored by extending it to single-phase turbulent pipe flow [11], which we described as the compromise in competition between viscous and inertial effects both formulated as extrema. We then made a daring prediction of its universality with respect to all complex systems [28, 29] based on these two successes in gas–solid and single-phase systems. The ability of the EMMS principle to describe multiscale systems promoted us to search for a general principle for all complex systems, that is, mesoscience, even as early as the 1990s [19, 28, 29], although without using such a term. However, we first had to convince the research community of the validity of the EMMS principle, which was a challenge. We spent many years validating the EMMS principle, which we did by verifying its principle, extending it to other systems, and using it to solve practical problems in both fundamental research and industrial applications.

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