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The Game Theoretical Approach for Multi-phase Complex Systems in Chemical Engineering*

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Abstract This paper explores the application of noncooperative game theory together with the concept of Nash equilibrium to the investigation of some basic problems on multi-scale structure, especially the meso-scale structure in the multi-phase complex systems in chemical engineering. The basis of this work is the energy-minimization-multi-scale (EMMS) model proposed by Li and Kwauk (1994) and Li, et al. (2013) which identifies the multi-scale structure as a result of 'compromise-in-competition between dominant mechanisms' and tries to solve a multi-objective optimization problem. However, the existing methods often integrate it into a problem of single objective optimization, which does not clearly reflect the 'compromise-in-competition' mechanism and causes heavy computation burden as well as uncertainty in choosing suitable weighting factors. This paper will formulate the compromise in competition mechanism in EMMS model as a noncooperative game with constraints, and will describe the desired stable system state as a generalized Nash equilibrium. Then the authors will investigate the game theoretical approach for two typical systems in chemical engineering, the gas-solid fluidization (GSF) system and turbulent flow in pipe. Two different cases for generalized Nash equilibrium in such systems will be well defined and distinguished. The generalize Nash equilibrium will be solved accurately for the GSF system and a feasible method will be given for turbulent flow in pipe. These results coincide with the existing computational results and show the feasibility of this approach, which overcomes the disadvantages of the existing methods and provides deep insight into the mechanisms of multi-scale structure in the multi-phase complex systems in chemical engineering.

Keywords Game theory, gas-solid fluidization, generalized Nash equilibrium, multi-phase complex systems, turbulent flow.

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1 Introduction

This paper explores the application of noncooperative game theory to chemical engineering and proposes a novel game theoretical approach to solve the problem on multi-scale structure in multi-phase complex systems modeled by the energy-minimization-multi-scale (EMMS) method[1, 2]. After formulating the problem as a noncooperative game with constraints, this paper introduces the concept of generalized Nash equilibrium (corresponding to the steady system sate), depending on two different typical systems in chemical engineering, i.e., the gas-solid fluidization system and the turbulent flow in pipe. The equilibrium solution coincides with the previous related numerical results in the literature.

With obvious significance, current process industry, especially in the developing countries, encounters serious problems with low energy conversion efficiency, high pollution and huge waste[3–5]. One of the reasons behind is lack of deep understanding on the movement, transition and reaction of matters during physical and chemical process in the multi-phase chemical engineering systems, especially on the meso-scale structure[6].

A typical example is the gas-solid fluidization (GSF) system, where at meso-scale, the particle cluster and gas move together and are interacted in a complex way. This leads to a widely recognized difficult problem to understand and compute stable states in such systems. In addition, coupling at meso-scale exists in many other systems. Deep understanding about the formation mechanisms of multi-scale structures in such systems may help to enhance the capability of improving equipment productivity and developing new technologies.

The EMMS model trying to reveal the internal principle in the multi-phase complex systems like the particle-fluid system in gas-solid fluidization was first proposed by Li[7]. To be specific, the multi-scale structure is considered to be a result of compromise-in-competition among different dominant mechanisms which should be identified in different complex systems. Different mechanisms have different individual extremum tendencies, which lead to the stability criterion for the system. Traditionally, the EMMS method was formulated mathematically as multi-objective optimization or multi-objective variational (MOV) problem[1, 2, 6], and was solved by transferring the problem into a single-objective one, which leads to heavy computing burden and uncertainty in choosing appropriate weighting factors. Furthermore, such a mathematical treatment is elusive in characterizing the essence of mechanisms to form multi-scale structures.

Although the EMMS model was firstly proposed to a solve the gas-solid fluidized systems, it has been successful in many other systems including gas-liquid systems and single-phase turbulent flows[2, 6].

This paper will revisit and dig the phenomenon and principle of compromise-in-competition between different dominant mechanisms in the EMMS model. As will be illustrated in this paper, this principle can be captured by the idea of noncooperative games. This appears to be a novel application of the idea of game theory.

Game theory, especially the noncooperative game theory, studies how agents make decisions given that everyone's payoff is influenced by actions of all others[8]. It has made great progress and impact in the last decades. A key concept is the well-known Nash equilibrium[9, 10], which

describes a possible stable state of the system, at which no agent will unilaterally deviate from its action.

Despite of the widespread applications of game theory in diverse fields like economics, sociology, politics, biology and military field, etc.[11, 12], to the best of our knowledge, the use of game theory to formulate the relationship among matters in science or technology has been rarely explored.

An initial step trying to investigate the 'compromise-in-competition' mechanism in EMMS model from a noncooperative game viewpoint was made in [13]. This game-theory-based approach will clearly capture the physical meaning of the problem and might supply a promising method to solve other related problems. This paper will further explore the approach on two typical multi-scale systems in chemical engineering, the gas-solid fluidization (GSF) system and turbulent flow in pipe.

By formulating the system as noncooperative game, the concept of generalized Nash equilibrium will be introduced, in which the influential factors for the mechanisms' objective are related or coupled, i.e., space of the objective's influential factors for each mechanism changes with the choice of strategy of the other mechanism. In the gas-solid fluidization system, the influential factors are strategies of mechanisms and the environment variables; in the turbulent flow, the influential factors are only strategies of mechanisms. This concept is different from the Nash equilibrium or related equilibrium concept[8] and a general theory as well as algorithms on such games require further investigation. For the specific GSF system, we will solve the general Nash equilibrium which include a dominant strategy for one mechanism by its special properties; the solution coincides with previous numerical results of chemical engineers without missing the physical meaning of the problem. For the turbulent flow system, we will supply a feasible method to solve the generalized Nash equilibrium, by which the search space for the problem can be reduced. Thus the game theoretical approach is believed to be a promising way to solve the EMMS model for multi-phase complex systems in chemical engineering.

The remainder of this paper is organized as bellow. Section 2 provides some necessary preliminaries for noncooperative game theory; Section 3 studies the game theoretical formulation and solution for generalized Nash equilibrium for GSF systems; Section 4 is about the system of turbulent flow in pipe; Section 5 concludes the paper.

2 Preliminary for Noncooperative Game Theory

The noncooperative game theory studies how rational players make decisions with the interactions between each other. There are two ways to describe a game: The strategic or normal form and the extensive form. The extensive form description of a game can explicitly model the timing of the players' decisions, which can be analyzed by the strategic form. Thus next we only introduce the strategic form of a game[8].

A noncooperative game in the strategic form constitutes three elements:

(i) The players (who are actually decision makes), denoted by P_i, $i = 1, 2, \cdots, n$, $n \geq 2$;

(ii) The pure strategy space S_i for each player P_i, and $s_i \in S_i$ denotes a specific strategy

for player P_i, while $s = (s_1, s_2, \cdots, s_n) \in S = \prod_i S_i$ is called a strategy profile of the players;

(iii) The utility function u_i for each player P_i, where $u_i = u_i(s)$ depends on the strategies of all players. This makes game theory different from optimization theory. Equally, u_i can be regarded as an objective function J_i, which will be optimized (maximized or minimized) by the player. Through this section, we assume that the players would like to minimize u_i.

When $\sum_i u_i(s) = 0, \forall s$, the game is called zero-sum game. This is the extreme case of the games and most games of interest are non zero-sum. Here we only consider the most basic assumptions, i.e., the players in the game are finite, rational and have complete and perfect information. This can be roughly understood as that all players know the structure of the game and they know that all of them know this. Then, given three elements of a game, what will be the outcome of the game? i.e., What strategies will all the players decide to choose? To predict this, the most important concept is Nash equilibrium.

Definition 2.1 The strategy profile $S^* = (s_1^*, s_2^*, \cdots, s_n^*)$ is called a Nash equilibrium of the game, if

$$u_i(s_i^*, s_{-i}^*) \leq u_i(s_i, s_{-i}^*), \quad \forall i, \forall s_i \in S_i, \tag{1}$$

in which $s_{-i} = (s_1, \cdots, s_{i-1}, s_{i+1}, \cdots, s_n)$ denotes the strategy profile of the players except P_i.

From the definition, at Nash equilibrium, the strategy of every player is the best response to the strategy profile of all the other players, thus no player would unilaterally deviate from the equilibrium. Thus Nash equilibrium defines a reasonable prediction for the games'outcome and players' behavior. Nash equilibrium is the key concept in modern game theory with an advantage that it exists in a broad class of games[9]. The definition above actually defines the pure strategy Nash equilibrium; to assure the general existence of Nash equilibrium, mixed-strategy Nash equilibrium needs to be defined.

A mixed strategy σ_i for player P_i is a probability distribution over pure strategies of P_i, i.e., $\sigma_i = (\sigma_i(s_i))_{s_i \in S_i}$, $\sum_{s_i \in S_i} \sigma_i(s_i) = 1$. Then the utility of the player P_i becomes

$$u_i(\sigma_1, \sigma_2, \cdots, \sigma_n) = \sum_{(s_1, s_2, \cdots, s_n) \in S} \left(\prod_{j=1}^{n} \sigma_j(s_j) \right) u_i(s_1, s_2, \cdots, s_n).$$

Then Nash proved the theorem below by using Kakutani's fixed point theorem[10]:

Every finite strategic form game has a mixed strategy Nash equilibrium.

To deal with more general and complicated games like dynamic game with incomplete information, there are many extensions and refinements of Nash equilibrium, like correlated equilibrium, subgame perfect Nash equilibrium, Bayesian equilibrium and so on. These concepts are refered to [8] for more details.

3 Game Theoretical Approach for GSF

3.1 EMMS Model for Gas-Solid Fluidization (GSF)

Fluidization is a unit operation applied widely in different industries. In circulating fluidized beds, particle clustering phenomenon exists and causes coexistence of dilute gas-rich and dense

particle-rich phases due to the increasement of gas velocity, which make it challenging to analyze the gas-solid interactions[14–16].

A gas-solid fluidization (GSF) system possesses heterogeneous structures, roughly consisting of dense and dilute phases with interaction at their interface. To describe such a system, eight parameters at three scales are necessary[6]:

(i) Particle scale: Voidage ε_f, superficial particle velocity U_{pf} and superficial fluid velocity U_f for the dilute phase and corresponding parameters ε_c, U_{pc} and U_c respectively for the dense phase.

(ii) Meso-scale: Cluster volume fraction f and cluster diameter d_{cl} are used to describe the interaction between the dense and dilute phases.

(iii) Global scale: Operating conditions (superficial gas velocity U_g and particle velocity U_p) and material properties (density ρ_p and diameter d_p for particles, and viscosity ν_f and density ρ_f for the fluid) are specified; average voidage ε needs to be deduced through calculation.

Then the system state can be defined to be $X = (\varepsilon_f, U_f, U_{pf}, \varepsilon_c, U_c, U_{pc}, f, d_{cl})$ since other parameters can be deduced by X. To solve the system state, equations involving the eight parameters in X are needed. According to fundamental physical laws, six conservation equations, called fundamental equations in EMMS model, are available[6]:

$$F_1(X) = m_c F_c f + m_i F_i - f(1-\varepsilon_c)(\rho_p - \rho_f)g = 0, \tag{2}$$

$$F_2(X) = (1-f)m_f F_f - (1-f)(1-\varepsilon_f)(\rho_p - \rho_f)g = 0, \tag{3}$$

$$F_3(X) = m_f F_f + \frac{m_i F_i}{(1-f)} - m_c F_c = 0, \tag{4}$$

$$F_4(X) = U_g - U_f(1-f) - U_c f = 0, \tag{5}$$

$$F_5(X) = U_p - U_{pf}(1-f) - U_{pc} f = 0, \tag{6}$$

$$F_6(X) = d_{cl} - \frac{g d_p \left[\frac{U_p}{1-\varepsilon_{\max}} - U_{mf} + \frac{\varepsilon_{mf} U_p}{1-\varepsilon_{mf}}\right]}{N_{st}\frac{\rho_p}{\rho_p - \rho_f}} - \left(U_{mf} + \frac{\varepsilon_{mf} U_p}{1-\varepsilon_m f}\right) g = 0. \tag{7}$$

In the above systems, the theoretical extreme value for the parameter $\varepsilon_{\max}$ is 1, which is usually taken as $\varepsilon_{\max} = 0.9997$ in actual computation. Other variables are physical constants or system variables, see [6].

Apparently, the system above with 6 equations and 8 parameters are not closed and calls for additional conditions. To this end, the EMMS model[2, 7] tried to build stability conditions by comprise in competition between two dominant mechanisms, which are identified for the specific system and will affect the system stability as well as structure resolution.

For GSF, there are two dominant mechanisms, which are the extremal tendencies for gas and solids. Concerning the gas, the extremal tendency can be expressed as to minimize energy consumption for suspending and transporting particles per unit volume[16]:

$$\begin{aligned} W_{st} = \frac{3}{4}\Bigg[& C_{dc}\frac{1-\varepsilon_c}{d_p}\rho_f U_{sc}^2 U_c f + C_{df}\frac{1-\varepsilon_f}{d_p}\rho_f U_{sf}^2 U_f (1-f) \\ & + C_{di}\frac{f}{d_{cl}}\rho_f U_{si}^2 U_f (1-f)\Bigg] \quad \to \min . \end{aligned} \tag{8}$$

Concerning the solids, the extremal tendency is to minimize average voidage[16]:

$$\varepsilon = \varepsilon_f(1-f) + \varepsilon_c f \quad \rightarrow \min . \tag{9}$$

Then the EMMS model claims that 'compromise in competition between the dominant mechanisms' defines the stability condition of the system. The parameters at different scales are correlated and three regimes are generally possible to appear depending on the extent of the relative dominance of the two mechanisms[6]:

(i) Particle-Dominated (PD) regime: When gas velocity is low, the influence of gas on system structure is negligible, so the system is exclusively PD, which can be described by

$$\varepsilon \rightarrow \min, \tag{10}$$

while $W_{st} \rightarrow \min$ is suppressed.

(ii) Particle-Fluid-Comprising (PFC) regime: With increasing dominance of gas over solids, the PD state is gradually suppressed while the Fluid-Dominated (FD) state is intensified, thus the mechanism $\varepsilon \rightarrow \min$ must compromise with $W_{st} \rightarrow \min$. The compromise in competition between them leads to complex mesoscale phenomena and the system may be conceptually described by

$$\begin{bmatrix} \varepsilon \\ W_{st} \end{bmatrix} \rightarrow \min . \tag{11}$$

(iii) Fluid-Dominated (FD) regime: When the dominance of $W_{st} \rightarrow \min$ increases to a critical value, $\varepsilon \rightarrow \min$ is completely suppressed and the FD state dominates the system. The system can be described by

$$W_{st} \rightarrow \min . \tag{12}$$

In the PFC regime, by physics, the parameter satisfies

$$\varepsilon_{mf} \leq \varepsilon_c \leq \varepsilon_{\max}, \tag{13}$$

where $\varepsilon_{mf} = 0.5$ is decided by physical characters of the GSF system.

The optimization problems in PD and FD regimes are regular. However, the optimization in PFC regime appears to be a multi-objective optimization problem. In the EMMS model, it is integrated into a single criterion

$$N_{st} = \frac{W_{st}}{(1-\varepsilon)\rho_p} \longrightarrow \min \tag{14}$$

by analyzing physics of the system.

The analytical treatment above has its own weakness. The correlation of cluster diameter needs to be improved to remove the uncertainty from $\varepsilon_{\max}$ based on experimental data and this problem is still unsolved, calling for fundamental research on the dynamic formation and dissolution of clusters. The game theoretical approach below might shed some light on it.

3.2 Game-Based Formulation and Solution for GSF

First, we note that the idea of 'comprise in competition of dominant mechanisms' is naturally similar to the noncooperative game theory. This inspires us to reconsider the problem from the prospective of game theory. Since the EMMS model must satisfy physical laws, we will be to consider games with constraints. Next we state a general formulation for such games.

Consider a system with n players making decisions in a game. The actions of players are denoted by a_i, which is from the action space $\mathcal{A}_i$ of player P_i. The action profile of all players is denoted by $a = (a_1, a_2, \cdots, a_n)$. The game is played in the environment which is denoted by $e \in E$, and it is influenced by actions of players, which is described as $e = e(a) : \prod_i \mathcal{A}_i \mapsto E$, where the mapping $e(a)$ cannot be analytically obtained often.

The objective function for each player to be minimized will not only depend on the action profile of the players a, but also depend on the environment e. Thus we have

$$J_i = J_i(e, a_i, a_{-i}),$$

where a_{-i} denotes the action profile of players other than that of the player P_i, i.e., $a_{-i} = (a_1, a_2, \cdots, a_{i-1}, a_{i+1}, \cdots, a_n)$. This is essentially different from utility in classical games[8] and will bring about different concept of equilibrium, which can be defined as below.

Definition 3.1 An action profile $a^* = (a_1^*, a_2^*, \cdots, a_n^*)$ is called generalized (pure) Nash equilibrium based on its environment if for any i, it satisfies

$$J_i(e(a_i^*, a_{-i}^*), a_i^*, a_{-i}^*) = \min_{a_i \in \mathcal{A}_i} J_i(e(a_i, a_{-i}^*), a_i, a_{-i}^*). \tag{15}$$

The generalized Nash equilibrium defined above is different from the concept of Nash equilibrium. The objective functions of mechanisms in (15) are related with both action profile a and environment $e(a)$, which cannot be written in the form of the objective functions in (1).

Concerning the GSF system in PFC regime, the two dominant mechanisms can be regarded as two players, with the respective parameters being their actions. To be specific, the extremal tendency of solids $\varepsilon \to \min$ is for mechanism or player P_1, and the extremal tendency of gas $W_{st} \to \min$ is for mechanism or player P_2. According to the physics in EMMS model, their actions are ε_c and ε_f respectively, which are independent with each other, i.e., $a_1 = \varepsilon_c$, $a_2 = \varepsilon_f$. All the other 6 parameters in the system state X in EMMS model are regarded as the environment and called environment state variables $e = (U_f, U_{pf}, U_c, U_{pc}, f, d_{cl})$, which are influenced by ε_c and ε_f according to the conservation equation (2).

According to the analysis in the section above, the objective function of mechanism P_1 is

$$J_1(e, a_1, a_2) = \varepsilon_f(1 - f) + \varepsilon_c f. \tag{16}$$

Similarly, the objective function of mechanism P_2 is

$$\begin{aligned} &J_2(e, a_1, a_2) \\ =&\frac{3}{4}\left[C_{dc}\frac{1-\varepsilon_c}{d_p}\rho_f U_{sc}^2 U_c f + C_{df}\frac{1-\varepsilon_f}{d_p}\rho_f U_{sf}^2 U_f(1-f) + C_{di}\frac{f}{d_{cl}}\rho_f U_{si}^2 U_f(1-f)\right], \end{aligned} \tag{17}$$

where $0.5 \leq \varepsilon_c, \varepsilon_f \leq 1, d_p \leq d_{cl}$. And the mechanisms P_1 and P_2 would like to to minimize their objective functions J_1 and J_2 respectively.

Assume that $(\varepsilon_c^*, \varepsilon_f^*)$ is the generalized Nash equilibrium based on environment, whose existence is assumed. Then, according to the definition, we have

$$J_1(e(\varepsilon_c^*, \varepsilon_f^*), \varepsilon_c^*, \varepsilon_f^*) \leq J_1(e(\varepsilon_c, \varepsilon_f^*), \varepsilon_c, \varepsilon_f^*). \tag{18}$$

By (16),

$$\frac{dJ_1(e(\varepsilon_c, \varepsilon_f^*), \varepsilon_c, \varepsilon_f^*)}{d\varepsilon_c} = f|_{(\varepsilon_c, \varepsilon_f^*)} + (\varepsilon_c - \varepsilon_f^*)\frac{\partial f}{\partial \varepsilon_c}\bigg|_{(\varepsilon_c, \varepsilon_f^*)}.$$

First, we have the physical fact that $0 < f < 1$ and $\varepsilon_c \leq \varepsilon_f$. On the other hand, by the physics in EMMS model, we have $\frac{\partial f}{\partial \varepsilon_c}|_{(\varepsilon_c, \varepsilon_f)} \leq 0$ (see [2]), Thus we get

$$\frac{dJ_1(e(\varepsilon_c, \varepsilon_f^*), \varepsilon_c, \varepsilon_f^*)}{d\varepsilon_c} > 0,$$

which means that the objective $J_1(e(\varepsilon_c, \varepsilon_f^*), \varepsilon_c, \varepsilon_f^*)$ increases with ε_c strictly. Remind (13), we know that to minimize $J_1(e(\varepsilon_c, \varepsilon_f^*), \varepsilon_c, \varepsilon_f^*)$, the mechanism P_1 must take $\varepsilon_c^* = \varepsilon_{mf} = 0.5$. Note that this strategy $\varepsilon_c^* = 0.5$ is a dominant strategy[8] for P_1, i.e., it is independent of P_2's choice of ε_f. Thus in the fundamental equations and the objective function J_2, the parameter ε_c can be regarded as a constant value $\varepsilon_c^* = 0.5$.

Now consider P_2. Given $\varepsilon_c^* = 0.5$, the corresponding objective function is

$$\begin{aligned} J_2 =& \frac{3}{4}\Bigg[C_{dc0}\left(\frac{1}{2}\right)^{-4.7}\frac{1}{2d_p}\rho_f(U_c - U_{pc})^2 U_c f \\ &+ C_{df0}(\varepsilon_f)^{-4.7}\frac{1-\varepsilon_f}{d_p}\rho_f\left(U_f - \frac{\varepsilon_f U_{pf}}{1-\varepsilon_f}\right)^2 U_f(1-f) \\ &+ C_{di0}(1-f)^{-4.7}\frac{f}{d_{cl}}\rho_f(U_f - 2\varepsilon_f U_{pc})^2(1-f)^2 U_f(1-f)\Bigg]. \end{aligned} \tag{19}$$

Apparently, the value of J_2 depends on both ε_f and the environment state variables $e = (U_f, U_{pf}, U_c, U_{pc}, f, d_{cl})$. Thus, to get the optimal strategy ε_f^* for minimizing J_2, P_2 equally needs to solve a conditional extreme value problem:

$$\begin{aligned} \min_{\varepsilon_f, e} \quad & J_2 \\ \text{s.t.} \quad & F_i(\varepsilon_f, e) = 0, \quad i = 1, 2, \cdots, 6; \\ & \varepsilon_f, e \geq 0. \end{aligned} \tag{20}$$

By writing all the variables out, we can see that in the above constrained optimization problem (20), there is an external variable U_g which can be regulated and controlled. Along with the change of U_g, the solution to the problem (20) will definitely change too. For each fixed U_g, the problem can be solved theoretically by Lagrangian multiplier method. Next, the optimization problem (20) is calculated numerically for the EMMS model with FCC catalyst/air

system, see [1]. The physical parameters needed during the optimization process are taken as below: $d_p = 54\mu$m, $\rho_p = 929.5$kg/m^3, $\varepsilon_{mf} = 0.5$, $U_{mf} = 0.002$m/s, $\rho_f = 1.1795$kg/m^3, $\mu_f = 1.8872*10^{-5}$kg/(m.s), $G_s = 50$kg/(m.s). Then, by computing ε_f^* numerically along with feasible U_g which can be controlled to take different values, we can build the relationship between U_g and the optimal solution ε_f^*, and the result is shown in Figure 1 as below.

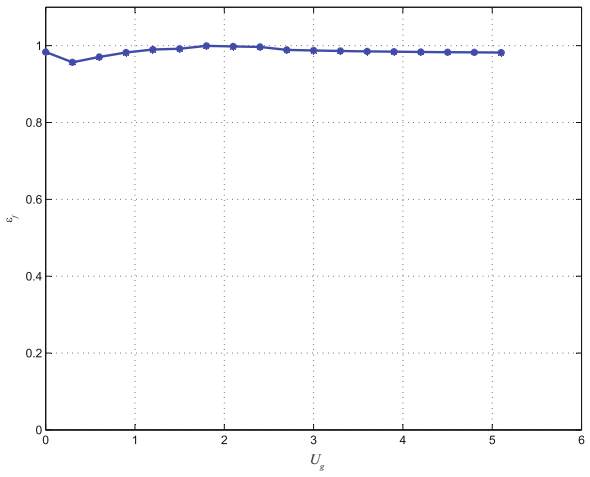

Figure 1 The relation between ε_f^* and U_g

From Figure 1, we can see that to minimize J_2, $\varepsilon_f^* \approx 1$, i.e., the theoretical value of $\varepsilon_{\max}$, which hardly changes with U_g.

Thus for the game formulated from the GSF system, we obtain the generalized Nash equilibrium to be $(\varepsilon_c^* = 0.5, \varepsilon_f^* = 1)$. And the environment state $e = (U_f, U_{pf}, U_c, U_{pc}, f, d_{cl})$ corresponding to Nash equilibrium can also be computed, which however changes with the specific value of U_g.

The result of generalized Nash equilibrium $(\varepsilon_c^* = 0.5, \varepsilon_f^* = 1)$ just coincides with the previous computational results of ε_f^* and ε_c^* which is shown in Figure 2. Figure 2 (see [1]) is obtained by solving the single-criterion optimization problem to compute the steady state with eight variables $X = (\varepsilon_f, U_f, U_{pf}, \varepsilon_c, U_c, U_{pc}, f, d_{cl})$ by general reduced gradient method (GRG). The abscissa axis also denotes the value of U_g.

In addition, if we make a rough use of the physical meanings of environment variables $e = (U_f, U_{pf}, U_c, U_{pc}, f, d_{cl})$ as in [13], then the influence of P_2's action ε_f to e is tiny and thus we can regard e as constants, then J_2 only depends on the middle term of (19), which is always non-negative and will reach its minimum value 0 at $\varepsilon_f^* = 1$.

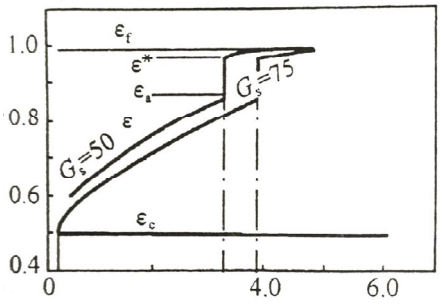

Figure 2 The previous computational results of ε_f^* and ε_c^* in [1]

Remark 3.2 The game theoretical formulation of the problem is not unique. Strategy space of each mechanism can be decided in different ways, leading to different understanding of the system and different difficulties in analysis. For specific systems, it seems worthy to explore the most suitable game model.

To sum up, in the EMMS model for the GSF system, two dominant mechanisms compromise in competition, which may be captured by the idea of game theory. This inspires us to formulate the problem to be a noncooperative game with constraints. For such games, we define the generalized Nash equilibrium based on environment in general. Then for the GSF system, we compute the generalized Nash equilibrium, which coincides with computational result obtained before. Furthermore, the formulation does not damage the physical meaning of the problem, and implies deeper understanding on the essence inside the emergence of multi-scale structures.

4 Game Theoretical Views for Turbulent Flow in Pipe

4.1 The Turbulent Flow in Pipe

The well-known Reynolds experiment[17] in 1883 revealed two distinct types of flow: Laminar flow and turbulent flow. In laminar flow, the fluid follows a clear and regular movement law. On the contrary, turbulent flow implies randomness or irregularity in time or space, and large scale swirls inside. So far, the general mechanism for turbulent flow is still an open and challenging scientific problem. Some review about four main theories to study turbulent flow are referred to [18].

In this paper we consider the simplest case: The turbulent flow in pipe. In this case, by physical experiment, the velocity with respect to the distance from the pipe center can be chosen as

$$u(r) = a_1\left[1 - \left(\frac{r}{R}\right)^{n_1}\right] + a_2\left[1 - \frac{r}{R}\right]^{1/n_2}, \tag{21}$$

where a_1, a_2 are respectively the weight factors of the non-turbulent and turbulent flows, n_1 and n_2 are integers to be decided, and R is radius of the pipe.

4.2 EMMS Model of Turbulent Flow

In chemical engineering, turbulent flow emerges often and interact with droplet, bubbles or particles in a complex way. That will greatly affect the chemical processes in multi-phase systems. On the other hand, turbulent and nonturbulent fluids (laminar flow) often coexist in the fluid. However, traditional turbulence models often neglect the laminar portion of the fluid, which leads to inaccuracies in modeling practical engineering flows.

To this end, [19] extended the idea of EMMS model to turbulent flow by taking the turbulent flow as a type of nonlinear non-equilibrium complex system. In the model, turbulent flow is thought as the result of the compromise in competition between viscosity and inertia, the two different dominant mechanisms in turbulent flow which come from their corresponding extremum tendencies. Then from that the turbulence stability criterion can be derived.

In the fluid flow, both the inertial and viscous forces are important to form complex turbulent flows[20]. When either viscosity or inertia dominates the system exclusively, there is no inhomogeneous flow structure formed. To be specific, when the viscous force dominates the system, the effect of inertia can be neglected and the flow is laminar flow, which is single phase; when both play roles in the system, an inhomogeneous flow structure occurs, and with increasing inertia a greater number of complex inhomogeneous flow structures form; when the effects of viscosity can be neglected in fluid flows, the flow is fully developed turbulent flow[21].

Now consider the extremum tendencies. If a flow is single-phase and dominated exclusively by viscosity, it aims to minimize the viscous mean shear dissipation rate[19]

$$\overline{W}_v = 2\pi \int_0^R r W_v(r) dr,$$

in which $W_v(r) = \mu\big(\frac{du(r)}{dr}\big)^2$, μ is the fluid viscosity.

By (21), we get

$$\frac{du(r)}{dr} = -n_1 a_1 \frac{r^{n_1-1}}{R^{n_1}} - \frac{a_2}{n_2 R}\left(1-\frac{r}{R}\right)^{\frac{1}{n_2}-1},$$

and thus

$$W_v(r) = \mu\left[\frac{du(r)}{dr}\right]^2 = \mu\left[-n_1 a_1 \frac{r^{n_1-1}}{R_1^n} - \frac{a_2}{n_2 R}\left(1-\frac{r}{R}\right)^{\frac{1}{n_2}-1}\right]^2.$$

Then we get

$$\begin{aligned}\overline{W}_v =& 2\pi\mu \int_0^{0.9999R} \left[n_1 a_1 \frac{r^{n_1-1}}{R_1^n} + \frac{a_2}{n_2 R}\left(1-\frac{r}{R}\right)^{\frac{1}{n_2}-1}\right]^2 r dr + 2\pi\mu \int_0^{0.9999R} \left[\frac{du(r)}{dr}\Big|_R\right]^2 r dr \\ =& 2\pi\mu\left[\frac{n_1 a_1^2}{2} + \frac{2n_1 a_1 a_2}{n_2}\int_0^{0.9999R} x^{n_1}(1-x)^{\frac{1}{n_2}-1} dx + \frac{a_2^2}{n_2^2}\int_0^{0.9999R} x(1-x)^{\frac{2}{n_2}-2} dx\right] \\ &+ 2\pi\mu 10000[a_1(1-0.9999^{n_1}) + a_2 0.0001^{1/n_2}]^2, \end{aligned} \tag{22}$$

where it is assumed that the area in the pipe from $0.999R$ to R is the viscous sublayer, which is very thin relative to R according to previous study[22].

If a flow is fully developed turbulent flow and dominated exclusively by inertia, it aims to maximize the total energy dissipation rate of turbulence[19]

$$\overline{W}_T = -2\pi R\overline{u}\mu \frac{du(r)}{dr}\Big|_R,$$

where $\overline{u}$ is the cross-sectional average fluid velocity

$$\begin{aligned}\overline{u} = \frac{2}{R^2}\int_0^R ru(r)dr &= \frac{2}{R^2}\int_0^R ra_1\left[1-\left(\frac{r}{R}\right)^{n_1}\right]dr + \int_0^R ra_2\left[1-\frac{r}{R}\right]^{1/n_2}dr \\ &= \frac{n_1a_1}{n_1+2} + \frac{2n_2^2a_2}{(n_2+1)(2n_2+1)}. \end{aligned} \tag{23}$$

Thus, we get

$$\begin{aligned}\overline{W}_T &= -2\pi R\mu\overline{u}\frac{du(r)}{dr}\Big|_R \\ &\approx 2\pi\mu R\frac{u(r)|_{0.9999R}-0}{R-0.9999R} \\ &= 2\pi\mu\overline{u}10000[a_1(1-0.9999^{n_1})+a_20.0001^{1/n_2}]. \end{aligned} \tag{24}$$

In its EMMS model, the turbulent flow is a result of compromise in competition between these two dominant mechanisms, leading to the stability criterion, which can be expressed as

$$\begin{bmatrix} \overline{W}_v \\ -\overline{W}_T \end{bmatrix} \to \min.$$

In an early work, Wang[22] decomposed $\overline{W}_T$ into the sum of $\overline{W}_v$ and the dissipation rate of fluctuation $\overline{W}_{te}$, i.e., $\overline{W}_T = \overline{W}_v + \overline{W}_{te}$, and thought the latter one decides the tendency of $\overline{W}_T$, thus the mechanism of turbulent flow becomes

$$\begin{bmatrix} \overline{W}_v \\ -\overline{W}_{te} \end{bmatrix} \to \min.$$

Apparently, the mechanism of turbulent flow above is a multi-objective variational (MOV) problem. As in EMMS model for GSF system, previous work in the field of chemical engineering changes the MOV problem to a single-objective problem. By introducing the weight factor $\alpha = \frac{\overline{W}_{te}}{\overline{W}_T}$ denoting the weight of inertia in turbulent flows, a single objective can be obtained to be

$$F = \overline{W}_{te} - \overline{W}_v = \alpha\overline{W}_T - \overline{W}_v \ \to \ \max. \tag{25}$$

However, α at the stable sate cannot be solved even it has a clear meaning in physics. To decide α, the most commonly used approach is to find the corresponding optimum parameters n_1, n_2, a_1, a_2 by computing optimum of F via choosing α ergodicly. Then the velocity of flow can be obtained and can be compared with the empirical formula. The α leading to the velocity which is most close to empirical formula is the desired α, under which the optimum of parameters n_1, n_2, a_1, a_2 have already been computed. Obviously, such an approach takes a big detour and results in heavy computing burden. Moreover, in physics, F is not as clear as $\overline{W}_v$ or $\overline{W}_{te}$.

4.3 The Game-Based Formulation and Solution for Turbulent Flow

Similar to our analysis in the GSF system, we can formulate the compromise in competition between viscosity mechanism and inertia mechanism in turbulent flow as a noncooperative game.

Here the game is between the viscosity and inertia mechanisms. The parameters n_1, n_2, a_1, a_2 constitute their strategies or actions (they are the same here), where the viscosity mechanism controls its action $S_1 = (a_1, n_1)$ and the inertia mechanism controls $S_2 = (a_2, n_2)$.

For the viscosity mechanism, it aims to minimize J_1; and for the inertia mechanism, it aims to minimize J_2; their respective objective functions are

$$J_1 = \overline{W}_v, \quad J_2 = -\overline{W}_{te}.$$

From the EMMS model described above, we get

$$\begin{aligned} J_1 &= 2\pi\mu\left[\frac{n_1 a_1^2}{2} + \frac{2n_1 a_1 a_2}{n_2}\int_0^{0.9999R} x^{n_1}(1-x)^{\frac{1}{n_2}-1}dx + \frac{a_2^2}{n_2^2}\int_0^{0.9999R} x(1-x)^{\frac{2}{n_2}-2}dx\right] \\ &\quad + 2\pi\mu 10000[a_1(1-0.9999^{n_1}) + a_2 0.0001^{1/n_2}]^2, \\ J_2 &= -(\overline{W}_T - \overline{W}_v), \end{aligned} \tag{26}$$

where $\overline{W}_T, \overline{W}_v$ are computed by (22) and (24).

First, note that there exist some physical constraints on the values of a_1, a_2, n_1, n_2. By (21) and (23), we can get a dimensionless value

$$\frac{u(r)}{\overline{u}} = a_1\left[1 - \left(\frac{r}{R}\right)^{n_1}\right] + a_2\left[1 - \frac{r}{R}\right]^{1/n_2}.$$

Obviously, a_1, a_2 must be dimensionless.

According to the physically evolutional process of the velocity of the flow in pipe, we have

$$1 \le \frac{u(r)}{\overline{u}}\Big|_{r=0} = a_1 + a_2 \le 2. \tag{27}$$

On the other hand, it has $\overline{u} = 1$, then we get

$$\frac{n_1 a_1}{n_1 + 2} + \frac{2n_2^2 a_2}{(n_2+1)(2n_2+1)} = 1. \tag{28}$$

Thus in this problem, the strategies (S_1, S_2) must satisfy two constraints (27) and (28), which can be resettled in a general form as

$$F_j(S_1, S_2) = 0,\ j = 1; \quad G_k(S_1, S_2) \le 0,\ k = 1, 2. \tag{29}$$

And the game becomes a noncooperative game with constraints on strategies (29). Thus we can define generalized Nash equilibrium with constraints as below:

Definition 4.1 $(S_1^*; S_2^*)$ is called the generalized Nash equilibrium of the game formulated above if for any i, it satisfies

$$J_i(S_i^*, S_{-i}^*) = \min_{S_i \in \mathcal{A}_i(S_{-i}^*)} J_i(S_i, S_{-i}^*),$$

where $\mathcal{A}_i(S^*_{-i}) = \{S_i : \ (S_i, S^*_{-i})$ satisfies (29)$\}$ denotes the strategy space of one mechanism given that its opponent chooses S^*_{-i}.

For this specific problem, we supply a possible method to solve Nash equilibrium $(a_1^*, n_1^*, a_2^*, n_2^*)$ below.

Step 1 Fix a_2 to be a reasonable value $\widehat{a_2}$ according to (27).

Step 1.1 Reformulate the feasible strategy for mechanism P_2 by (29) to be a function $n_2^*(a_1, n_1)$, which is just a singleton given the opponent's strategy a_1, n_1.

Step 1.2 Substitute $n_2^*(a_1, n_1)$ into J_1 and solve the optimization problem with constraints of P_1, denote the solution by $(\widehat{a_1^*}, \widehat{n_1^*})$.

Step 1.3 Check whether the strategy profile $(\widehat{a_1^*}, \widehat{n_1^*}; \widehat{a_2}, n_2^*(\widehat{a_1^*}, \widehat{n_1^*}))$ is a Nash equilibrium.

Step 2 Change to another a_2 and back to Step 1.

The method above will avoid choosing α in (25). Additionally, we only need to find a suitable a_2, (whose range can be narrowed by J_1) rather than choosing optimal a_1, n_1, n_2 ergodicly[22]. Thus potentially this method can considerably reduce the computation cost. However, we must note that the existence and uniqueness of generalized Nash equilibrium in the game above are open.

Remark 4.2 Note that the game models for GSF system and for turbulent flow are different. Surely this difference comes from the different features of the specific systems. From the view of game theory, in the game for GSF system, the influential factors beside strategies of mechanisms are described as environment which is hardly analytically expressed by the strategy profile, while the strategy space of each other is still independent. However, in the game for turbulent flow in pipe, the strategy spaces of mechanisms are correlated, i.e., if one mechanism changes his strategy, the space of available strategy for the other mechanism will change too. Thus in both cases, the influential factors for the mechanisms' payoffs are correlated or coupled, i.e., space of the payoff's influential factors for each mechanism changes with the choice of the other mechanism's strategy. Both of them are well defined in this paper and are different from classical game models. There is no doubt that more general cases exist and make sense. Thus, a great challenge on analysis and algorithms for generalized Nash equilibrium is posed too.

5 Conclusions

The understanding of the mechanisms and evolution of multi-scale structures in multi-phase complex systems is a fundamental problem in chemical engineering. This paper has made an attempt to apply the idea of noncooperative game theory to the energy-minimization multi-scale (EMMS) model. We formulate the 'compromise-in-competition' between the dominant mechanisms as a noncooperative game with constraints, where the stable system state corresponds naturally to a generalized Nash equilibrium. This paper investigates this game theoretical formulation and its solution for two typical multi-phase complex systems in chemical engineering, i.e., the gas-solid fluidization system and turbulent flow, and shows the feasibility of this novel idea and approach. Furthermore, the concepts of generalized Nash equilibrium in these two systems are distinguished, while both of which are well defined.

Further investigation is necessary in the future, including the verification of this game theoretical approach to other multi-phase complex systems in chemical engineering like gas-liquid systems. Important further work also include the investigation of general theory and algorithms for generalized Nash equilibrium in noncooperative game with constraints.

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