CHINA PARTICUOLOGY Vol. 1, No. 1, 7-12, 2003

CHARACTERISTIC DIMENSIONLESS NUMBERS IN MULTI-SCALE AND RATE-DEPENDENT PROCESSES

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Abstract Multi-scale modeling of materials properties and chemical processes has drawn great attention from science and engineering. For these multi-scale and rate-dependent processes, how to characterize their trans-scale formulation is a key point. Three questions should be addressed:

- How do multi-sizes affect the problems?
- How are length scales coupled with time scales?
- How to identify emergence of new structure in process and its effect?

For this sake, the macroscopic equations of mechanics and the kinetic equations of the microstructural transformations should form a unified set that be solved simultaneously.

As a case study of coupling length and time scales, the trans-scale formulation of wave-induced damage evolution due to mesoscopic nucleation and growth is discussed. In this problem, the trans-scaling could be reduced to two independent dimensionless numbers: the imposed Deborah number $De^*=(ac^*)/(LV^*)$ and the intrinsic Deborah number $D^*=(n_N{}^*c^{*5})/V^*$, where a, L, c^*, V^* and $n_N{}^*$ are wave speed, sample size, microcrack size, the rate of microcrack growth and the rate of microcrack nucleation density, respectively. Clearly, the dimensionless number $De^*=(ac^*)/(LV^*)$ includes length and time scales on both meso- and macro- levels and governs the progressive process. Whereas, the intrinsic Deborah number D^* indicates the characteristic transition of microdamage to macroscopic rupture since D^* is related to the criterion of damage localization, which is a precursor of macroscopic rupture. This case study may highlight the scaling in multi-scale and rate-dependent problems.

Then, more generally, we compare some historical examples to see how trans-scale formulations were achieved and what are still open now. The comparison of various mechanisms governing the enhancement of meso-size effects reminds us of the importance of analyzing multi-scale and rate-dependent processes case by case.

For multi-scale and rate-dependent processes with chemical reactions and diffusions, there seems to be a need of trans-scale formulation of coupling effect of multi-scales and corresponding rates. Perhaps, two trans-scale effects may need special attention. One is to clarify what dimensionless group is a proper trans-scale formulation in coupled multi-scale and rate-dependent processes with reactions and diffusion. The second is the effect of emergent structures and its length scale effect.

Keywords multi-scale, rate-dependent, Deborah number

Introduction

Recently, multi-scale modeling of materials properties and chemical processes has drawn great attention from science and engineering. For example, Kwauk & Li (2000) pointed out the significance of "three transfers plus one reaction" on multi-scales in process engineering and proposed an energy-minimization multi-scale model. According to them, there are three levels in process engineering: microscopic phenomena in individual particle and its surface; mesoscopic in particle clusters and macroscopic in reactors. The Center for Simulation of Dynamic Response of Materials and Materials and Process Simulation Center (MSC) at California Institute of Technology are carrying out full physics full chemistry multi-scale modeling in two closely relevant key applications: solid dynamics such as plastic deformation and failure in metals and high explosives such as chemical response to shock loading in high-energy material. These are two closely related multi-scale problems, for example see Goddard et al. (2000).

For chemical engineering, "chemical engineers have had years of experience in scaling up chemical reactors from laboratory to pilot to full-production scale. One such methodology involves the use of dimensionless numbers or groups that describe the system's behavior. These numbers show the relative importance of one physical phenomenon versus another and appear naturally when the governing equations that describe the conservation of momentum, energy and mass and their respective boundary conditions are nondimensionalized. Dimensionless groups can be used as a guide for scale-up even when direct numerical simulation is possible" (Economou et al., 1998). However, for multi-scale and rate-dependent processes, nondimesionalization is not so trivial as traditional processes, owing to their multi-scale nature in both space and time. Additionally, the differences in scales are usually more than one order, for instance, mesoscopic grains (noted by l) are in the order of micron whereas the sample size (noted by L) is usually greater than centimeter. Noticeably, the size ratio $R=l/L$ is very small, about 10^{-3} or 10^{-4}. Provided the effects on small scales can be averaged and represented by a parameter on a larger scale, the multi-scale problem can be decoupled and then treated by embedded calculations, etc. This is relatively easy. Otherwise, the coupling effect of length scales becomes a key point in the problem, for instance, how the small size ratio R affect the macroscopic process.

It is well known that size-independence, i.e. geometrical similarity, will be violated provided gravity, rate-effect or intrinsic length scale play significant role in concerned problems. For instance, the linearly enlarged bones but with constant strength σ_s (the supporting force ~ $\sigma_s L^2$) can only support the enlarged body weight (~$\rho g L^3$) up to a limiting size $L_c \sim \sigma_s/(\rho g)$. This is the effect of gravity, with no business of multi-scale or rate-effect. However, in multi-scale problems, scaling of interest is the combination of macroscopic size L and intrinsic mesoscopic sizes l and its effect on macroscopical behavior. Apart from these prescribed characteristic length scales, some new structures, like band-like structure, may emerge during the course of a process. This may greatly enhance the complexity of process engineering problems.

Not only the geometrical similarity, but dynamic and chemical similarity should be taken into account too, for instance, the rate-dependent effect. As the great ancient Greek thinker Heraclitus said "$\tau\alpha\ \pi\alpha\nu\tau\alpha\ \rho\varepsilon\iota$", meaning "everything flows". More than that, there might be various time-scales involved simultaneously in a concerned problem in process engineering. Even early in the Bible, the prophetess Deborah sang, "The mountains flowed before the Lord". It implies that the mountains moved on their own time scales rather than the Lord's time scale. Accordingly, the relevant time scales in mesoscopic processes would lead to unexpected constitutive rate-effects. In other words, there might be several length and time scales on various levels in process engineering we need to deal with, which may critically govern the scaling in these multi-scale and rate-dependent problems.

Therefore, for these multi-scale and rate-dependent processes, how to characterize their trans-scale formulation is a key point. For this, Barenblatt (1992) made a very significant statement in his closing plenary lecture at the 18th International Congress of Theoretical and Applied Mechanics. He said that in the mathematical models of the governing influence of the variations of the material structure on the macroscopic behavior of bodies, the macroscopic equations of mechanics and the kinetic equations of the microstructural transformations should form a unified set that be solved simultaneously.

Furthermore, since the fifties of the last century, a number of scientists in various trades, including Barenblatt, supposed that Deborah number De be the proper measure of the coupling effect of macroscopic parameter and microstructual transformation. Deborah number is a dimensionless number defined as follows

$$De = \frac{t_r(\text{meso-relaxation})}{t_i(\text{macro-imposed})}\,, \tag{1}$$

where t_r is the relaxation time scale of mesoscopic kinetics and t_i is the macroscopically imposed time scale. Certainly, this independent dimensionless number gives an indication of the relevant importance of the two time scales. However, one can immediately notice that Deborah number alone can not characterize the multi-scale phenomena, because of the absence of the size ratio.

Now, there are three key questions in these multi-scale and rate-dependent processes:

- How do the multi-sizes (like $R=l/L \ll 1$) affect the problems?
- How are the length scales coupled with time scales (like t_r and t_i)?
- How to identify emergence of new structure in process and its effect?

In this paper, as a case study of coupling length and time scales, the trans-scale formulation of damage evolution due to mesoscopic nucleation and growth is discussed. In this problem, the trans-scaling could be reduced to two independent dimensionless numbers: the imposed Deborah number and the intrinsic Deborah number. Both of them govern the progressive trans-scale process and its characteristic transition to macroscopic rupture. This case study may highlight the scaling in multi-scale and rate-dependent problems in process engineering. Then, more generally, we compare some historical examples to see how the trans-scale or rate-dependent formulations were achieved and what are still open now.

Dimensionless Trans-Scale Formulation of Damage Evolution

Because of the similarity between materials failure and process engineering, in this section we briefly examine damage evolution as a case study of multi-scale and rate-dependent process. Generally speaking, a unified set of macroscopic equations of continuum mechanics and mesoscopic kinetic equations (similar to reaction) could be written (Bai et al., 2002b):

$$\frac{\partial \rho}{\partial t} + \boldsymbol{v}\cdot\frac{\partial \rho}{\partial \boldsymbol{x}} + \rho\cdot\frac{\partial \boldsymbol{v}}{\partial \boldsymbol{x}} = 0\,, \tag{2}$$

$$\frac{\partial \boldsymbol{v}}{\partial t} + \boldsymbol{v}\cdot\frac{\partial \boldsymbol{v}}{\partial \boldsymbol{x}} = \rho^{-1}\cdot\frac{\partial \boldsymbol{\sigma}}{\partial \boldsymbol{x}}\,, \tag{3}$$

$$\frac{\partial (e-q)}{\partial t} + \boldsymbol{v}\cdot\frac{\partial (e-q)}{\partial \boldsymbol{x}} = \rho^{-1}\cdot\boldsymbol{\sigma}\cdot\frac{\partial \boldsymbol{v}}{\partial \boldsymbol{x}} - \rho^{-1}\cdot\frac{\partial \boldsymbol{h}}{\partial \boldsymbol{x}}\,, \tag{4}$$

$$\frac{\partial n}{\partial t} + \frac{\partial (n\cdot A)}{\partial c} + \frac{\partial (n\cdot \boldsymbol{v})}{\partial \boldsymbol{x}} = n_N\,. \tag{5}$$

The first three equations (2-4) are mass, momentum and energy balances on macroscopic level respectively. As usual, the symbols in the three equations, t, $\boldsymbol{x}$, ρ, $\boldsymbol{v}$, $\boldsymbol{\sigma}$, e, q and $\boldsymbol{h}$ are time, macroscopic coordinates, density, flow velocity vector, stress tensor, energy density, heat, and heat flux respectively. The last equation (5) addresses the balance of the number density of microdamage n in phase space $\{c, \boldsymbol{x}\}$, where c is the size of microdamage, equivalent to the above-mentioned mesoscopic length scale l. In this equation there are two mesoscopic kinetics: nucleation rate of microdamage number density n_N and average growth rate of microdamage A, respectively.

In order to understand the role of dimensionless number in this multi-scale and rate-dependent process easily, we turn to its one-dimensional version (ignoring energy equation for the time being):

$$\frac{\partial \varepsilon}{\partial t} = \frac{\partial v}{\partial x} \ , \quad (6)$$

$$\rho_0 \frac{\partial v}{\partial t} = \frac{\partial \sigma}{\partial x} \ , \quad (7)$$

$$\frac{\partial D}{\partial t} + \frac{D}{1+\varepsilon}\frac{\partial v}{\partial x} = f \ , \quad (8)$$

where t and x are temporal and spatial independent variables respectively; v, ε, σ and D are velocity, strain, stress and continuum damage of representative element respectively. Noticeably, f is dynamic function of damage (DFD), which is the agent bridging macroscopic mechanical field and mesoscopic kinetics of damage (Bai et al., 2002a),

$$f = \int_0^\infty n_N(c;\sigma)\cdot\tau(c)\cdot dc + \int_0^\infty \{n_N(c_0;\sigma)\int_{c_0}^{c_f}\tau'(c)\cdot dc\}\cdot dc_0, \quad (9)$$

where τ is the failure volume of an individual microdamage with current size c, c_0 is the nucleation size of microdamage and c_f is the moving front of microdamage population

$$t = \int_{c_0}^{c_f} \frac{dc}{V(c,c_0;\sigma)} \ , \quad (10)$$

where V is mesoscopic growth rate of microdamage number density in phase space $\{c, c_0\}$.

Table 1 lists all eight parameters and independent variables involved in the problem, with their corresponding dimensions. L, T and M are the notations of the dimensions of length, time and mass, respectively.

Table 1 Parameters and their dimensions in damage evolution

Entity		Notation	Dimension
Macro-Parameters	sample size	L	L
	material density	ρ	$M\cdot L^{-3}$
	sound speed	a	$L\cdot T^{-1}$
	constitutive stress (like yield strength)	σ_Y	$M\cdot L^{-1}\cdot T^{-2}$
	impact velocity	v_f	$L\cdot T^{-1}$
Meso-Parameters	nucleation rate of microcrack density	$n_N{}^*$	$L^{-4}\cdot T^{-1}$
	growth rate of microcrack	V^*	$L\cdot T^{-1}$
	microcrack size	c^*	L

In light of π theorem in dimensional analysis, the eight meso- and macroscopic parameters could form five independent dimensionless numbers, see Table 2. Then, the dimensionless equations are

$$\frac{\partial \varepsilon}{\partial \bar{t}} = M\cdot\frac{\partial \bar{v}}{\partial \bar{x}} \ , \quad (11)$$

$$\frac{\partial \bar{v}}{\partial \bar{t}} = S\cdot\frac{\partial \bar{\sigma}}{\partial \bar{x}} \ , \quad (12)$$

$$\frac{\partial D}{\partial \bar{t}} + \frac{D}{1+\varepsilon}\frac{\partial \bar{v}}{\partial \bar{x}} = De^{-1}\cdot\bar{f} \ , \quad (13)$$

where the dimensionless variables are:

independent variables:

$$\bar{t} = (at)/L \ , \quad (14)$$

$$\bar{x} = x/L \ ; \quad (15)$$

dependent variables:

$$\bar{v} = v/v_f \ , \quad (16)$$

$$\bar{\sigma} = \sigma/\sigma_Y \ , \quad (17)$$

$$\bar{f} = f/(n_N{}^* c^{*4}) \ . \quad (18)$$

Table 2 Macro-, meso- and trans-scale dimensionless numbers in damage evolution

	Dimensionless number	Expression
Macroscopic dimensionless numbers	Mach number M	$M = v_f/a$
	Damage number S	$S = \sigma_Y/(\rho a v_f)$
Mesoscopic dimensionless numbers	Intrinsic Deborah number D^*	$D^* = (n_N{}^* c^{*5})/V^*$
Trans-scale dimensionless numbers	Imposed Deborah number De^*	$De = a/(L n_N{}^* c^{*4})$ or $De^* = (ac^*)/(LV^*)$
	Ratio of length scale R	$R = c^*/L$

Three significant aspects in the formulation should be noted here. The first is that the five dimensionless numbers can be cataloged into three groups: Mach number M and damage number S are macroscopic ones; the intrinsic Deborah number D^* is mesoscopic and Deborah number De and length ratio R are trans-scaled. But contrary to common sense, the straightforward length ratio $R=c^*/L$ does not appear in the associated dimensionless equations. We will interpret this latter. Second, all dimensionless variables are not only dimensionless but also normalized, namely they are all in $O(1)$, except for strain ε and damage D, which are dimensionless themselves and usually small. So, in principle, the magnitude of the terms in the equations can be estimated according to the dimensionless numbers preceding them in the equations. Apart form the two familiar macroscopic dimensionless number M and S, the trans-scale dimensionless number, Deborah number De, plays a key role in the trans-scale and rate-dependent formulation. Finally, the transition of microdamage evolution to macroscopic rupture can be characterized by damage localization as follows,

$$\frac{\partial}{\partial t}\left(\frac{\partial D}{\partial x}\right)\Big/\frac{\partial D}{\partial x} \geqq \frac{\partial D}{\partial t}\Big/D \ . \quad (19)$$

It has been derived that the critical damage D_L of the localization transition can be represented by the intrinsic Deborah number D^* (Bai et al., 2002a; Bai et al., 2002b).

In summary, in the multi-scale and rate-dependent process, Deborah number De (trans-scaled) and intrinsic Deborah number D^* (mesoscopic), rather than length ratio

R, play governing roles. Thus, what is the underlying mechanism?

As a matter of fact, in this case study there are three time scales: the macroscopically imposed time scale $t_i=L/a$, mesoscopic nucleation time scale $t_N=(n_N*c*^4)^{-1}$ and mesoscopic growth time scale $t_V=c*/V*$. More importantly, the competitions among the three rate-processes, represented by the ratios of the time scales, govern the whole multi-scale and rate-dependent process. Actually, the ratios of the three time scales ARE the three dimensionless numbers: two Deborah numbers De and $De*$ and intrinsic Deborah number $D*$, see Table 3. The size effect, namely the effect of size ratio R, should be included in the time ratios, either Deborah number De or $De*$.

In one word, physically, this damage evolution is a rate-governed process and the competition among the rates of various processes governs the whole process. The effect of mesoscopic size on macroscopic damage is mainly due to the enhancement of meso-size effect by rate-processes.

Table 3 Characteristic time scales and dimensionless numbers in three processes in damage evolution

	Characteristic time scales		
	Imposed time scale	Nucleation time scale	Growth time scale
	$t_i=L/a$	$t_N=(n_N*c*^4)^{-1}$	$t_V=c*/V*$
Deborah numbers indicating relative importance of three processes			
Meso- vs. Macro-processes		$De=t_N/t_i=a/(Ln_N*c*^4)$	$De*=t_V/t_i=(ac*)/(LV*)$
Two meso-processes			$D*=t_V/t_N=(n_N*c*^5)/V*$

Table 4 Comparison of some mechanisms of enhancement of meso-size effects

Examples	Meso-scale parameter	Mechanism of enhancement	Trans-scale expression
Dislocation-Plasticity	Burgers vector b	Total of dislocations $N=\rho L^2$	$(b\rho u)\ \dot{\gamma}\approx O(1)$
Boundary Layer	BL thickness δ	Viscosity ν	$(\delta\sqrt{Re})/L\approx O(1)$
Damage Evolution	Microdamage size $c*$	Competition of rate-processes	$De*=(ac*)/(LV*)\approx O(1)$

Note: in the Table L, b, ρ, N, u and $\dot{\gamma}$ (second row); δ, ν and Re (third row) are macroscopic size, Burgers vector, dislocation density, total dislocation, dislocation velocity, shear strain rate, boundary layer thickness, viscosity and Reynolds number, respectively.

Discussions on Mechanisms Governing Enhancement of Meso-Size Effects

In fact, the mechanisms governing the enhancement of meso-size effects can vary from case to case, not only the above-mentioned competitions among macroscopically imposed and mesoscopically intrinsic rate-processes. Table 4 lists a comparison of some examples of various mechanisms. The straightforward way for mesoscopic structures to affect macroscopic behavior is the sum of mesoscopic elements. Plasticity resulting from dislocation motion, characterized by meso-scale Burgers vector b, is a most impressive example, see the second row of Table 4. In this case, continuum shear strain rate is proportional to the production of dislocation density, dislocation velocity as well as Burgers vector. Another classical example of size effect is boundary layer. Although boundary layer is still a macroscopic phenomenon, it is treated as a trans-scale problem here, because its thickness is much less than sample size L and it is an emerging small-size structure, which enlightens other problems. In this case the reason why the thin boundary layer can appear and affect macroscopic flow is due to the high viscosity resistance in boundary layer, see the third row of Table 4. So, the comparison of various mechanisms governing the enhancement of meso-size effects reminds us of the importance of analyzing multi-scale and rate-dependent processes in accordance with governing mechanisms.

With reaction and diffusions (mass diffusion, viscosity, i.e. momentum diffusion, and energy or heat diffusion), multi-scale and rate-dependent processes become much more complicated. Apart from geometric and dynamic similarities, chemical similarity should be taken into account. Chemical similarity alludes to maintaining the same mass transfer and chemical reaction characteristics as in the smaller system. The most important dimensionless numbers describing mass transport and chemistry are the Damköhler number Da and the Thiele modulus ϕ (Economou et al., 1998).

For the similarity conditions of chemical reactions, Damköhler introduced four dimensionless numbers. Essentially, The Damköhler number Da describes the relative importance of the rate of species production or loss relative to the rate of mass transfer away from the source. For example, Damköhler number I represents the ratio of number of moles transformed chemically over number of moles supplied by flow, or

$$I\equiv(UL)/(wC_A)\,, \tag{20}$$

where U, L, w and C_A are reaction rate, macroscopic length, flow velocity and concentration, respectively (Grassmann, 1971; Feng, 1989). In this formulation, only macroscopic length scale L appears and the effect of microscopic chemical reactions is condensed into the parameter of reaction rate U. Hence, the trans-scale feature in the multi-scale and rate-dependent processes is decoupled in this formulation, for instance, mesoscopic particle size of reactant r_0 does not appear in the formulation. So far, we wonder whether or not there is a trans-scale dimensionless parameter, like the Deborah number in damage evolution, governing the multi-scale processes with reaction and diffusion. Also, it is not clear what dimensionless group is a proper trans-scale formulation (if it is really needed) in the multi-scale and rate-dependent processes in chemical engineering.

But, one feature might be really significant in the processes with reaction and diffusions, either mass diffusion, viscosity or heat diffusion. That is the effect of emergent structures and its length scale. It is well known that a steady layer structure may emerge in the process, where both source and diffusion are in force (Holland, 1998). In general, the governing equation of production-diffusion is

$$\frac{\partial Z}{\partial t} = D_{\rm i}\frac{\partial^2 Z}{\partial x^2} + S_0 \,, \tag{21}$$

where Z is a dimensionless variable, $D_{\rm i}$ is diffusion coefficient and S_0 is corresponding source term. When approaching a steady state, a band-like structure with characteristic width $l_{\rm e}$ may emerge,

$$l_{\rm e} \approx \sqrt{D_{\rm i}/S_0} \,. \tag{22}$$

Shear bands in thermo-plastic deformation with heat diffusion is a typical example (Bai & Dodd, 1992). The thickness of the emergent band-like structure is

$$\delta \approx \sqrt{(\lambda\theta^*)/(\beta\tau^*\dot{\gamma}^*)} \,, \tag{23}$$

where λ, θ^* and $\beta\tau^*\dot{\gamma}^*$ are heat conductivity, characteristic temperature and heat source due to plastic work, in which β, τ^* and $\dot{\gamma}^*$ are the fraction of plastic work converted into heat, shear stress and shear strain rate, respectively. Shear band emerging in metallic glass by void diffusion reported recently is the other example of this kind (Huang et al., 2002).

The Thiele modulus ϕ describes the relative importance of surface reaction relative to their ability to diffuse,

$$\phi = r_0\sqrt{(kC_{\rm Ai}^{m-1})/D_{\rm i}} \,, \tag{24}$$

where r_0 is the radius of a spherical particle, k is reaction rate constant, $C_{\rm Ai}$ is surface concentration, $D_{\rm i}$ is diffusion coefficient and m is the order of reaction. Clearly, in the Thiele modulus, there is a microscopic length scale, individual particle radius r_0, but not macroscopic size L or any mesoscopic length scales. So, contrary to macroscopic dimensionless number, the Damköhler number Da, the Thiele modulus is more or less a microscopic number.

More importantly, the Thiele modulus does provide some important information on emergent length-scale effect. As a matter of fact, the definition of the Thiele modulus ϕ indicates the competition of the microscopical particle size r_0 and an emergent length scale l_0,

$$l_0 = \sqrt{D_{\rm i}/(kC_{\rm Ai}^{m-1})} \,. \tag{25}$$

However, either the Damköhler number or the Thiele modulus does not touch the effect of particle clusters. So, if there is a coupling effect of three levels, namely microscopic individual particle; mesoscopic particles clusters and macroscopic reactors in process engineering, we should introduce the effect of particle clusters. Maybe, there is a trans-scale dimensionless group governing multi-scale phenomena in process engineering involving particles.

In summary, for multi-scale and rate-dependent processes with chemical reactions and diffusions, at least two trans-scale effects may need special attention. One is to clarify what dimensionless group is a proper trans-scale formulation in the coupled multi-scale and rate-dependent processes with chemical reactions and diffusions. The second is that the effect of emergent structures and its length scale effect should be taken into the trans-scale formulation.

Concluding Remarks

From the above examples, the following remarks are pertinent.

(1) For trans-scale formulation of damage evolution, there are several length scales and time scales on meso- and macroscopic levels. The length scales are microcrack size at meso-scale and the sample size on macro-level, whereas the time scales are nucleation and growth rates of microcracks on meso-level and the imposed loading duration on macro-level. The connection between the two levels is usually based on non-linear coupling of stress field and the population of microcracks. So, a proper approach to the problem is the associated equations of continuum, momentum and microdamage evolution. There is one trans-scale dimensionless number: the imposed Deborah number $De^* = (ac^*)/(LV^*)$, which characterizes the multi-scale and rate-dependent process.

(2) In general, statistical mechanics and corresponding trans-scale closed formulation might be proper approaches to multi-scale and rate-dependent processes. When the time taken by a kinetic process on meso-scales becomes comparable with the time taken by imposed process on macro-scale, such a mesoscopic kinetics becomes important on macroscopical level. Otherwise the meso-kinetics can be treated by adiabatic approximation.

(3) For multi-scale and rate-dependent processes with chemical reactions and diffusions, the Damköhler number and the Thiele modulus represent some scale effects. However, there seems to be a need of trans-scale formulation of coupling effect of multi-scales and corresponding rates. Perhaps, two trans-scale effects

may need special attention. One is to clarify what dimensionless group is a proper trans-scale formulation in the coupled multi-scale and rate-dependent processes with chemical reactions and diffusions. The second is the effect of emergent structures and its length scale effect.

Acknowledgment

This work is granted by the National Natural Science Foundation of China (NSFC No. 10172084) and Major State Research Project G200007735.

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Manuscript received February 26, 2003 and accepted March 26, 2003.