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PRESENTATION SLIDES: Analytical Multi-Scale Methodology for Fluidization Systems - Retrospect and Prospect

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Fluidization XII

Analytical Multi-Scale Methodology for Fluidization

---- from a simple idea to industrial application

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Challenge
↓
Strategy
↓
Progress
- Verification
- Solution
- Extension
- Application
  - *CFD*
  - *Industry*
  - *Future*
- Limitation

↓
Conclusion

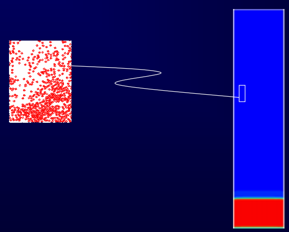
2

Challenge

3

1. Structure Heterogeneity

Local   Axial / Radial

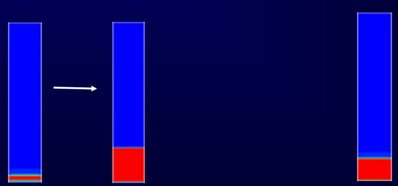


4

2. State Multiplicity

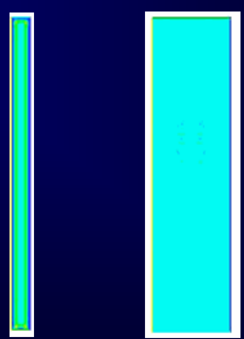
Jump Change (choking)
With slight change of operation condition

Co-existence
At a critical condition



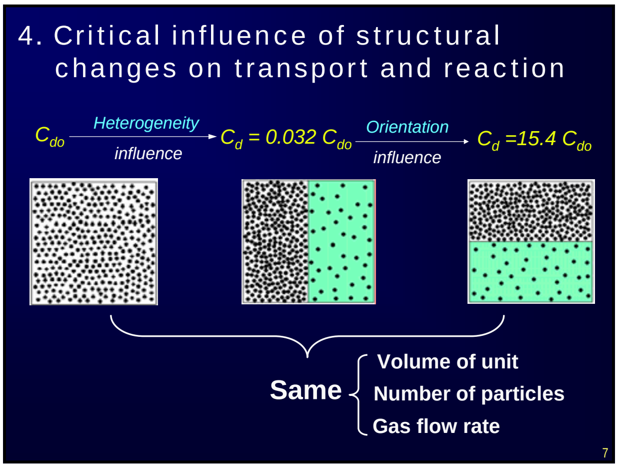
5

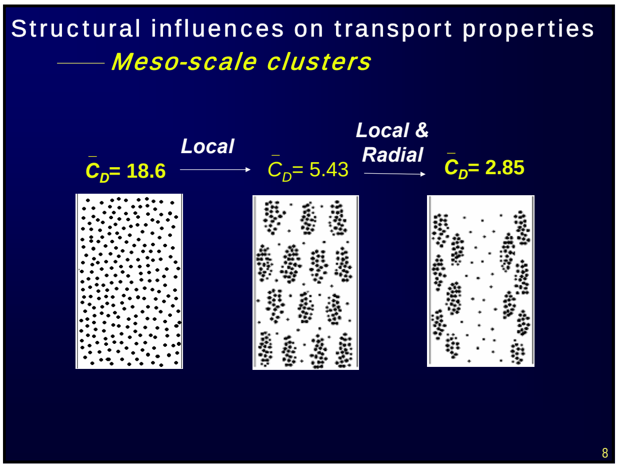
3. Scale-up Effect

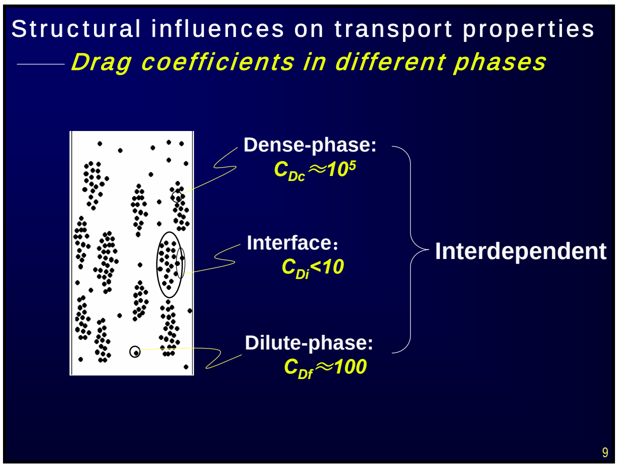


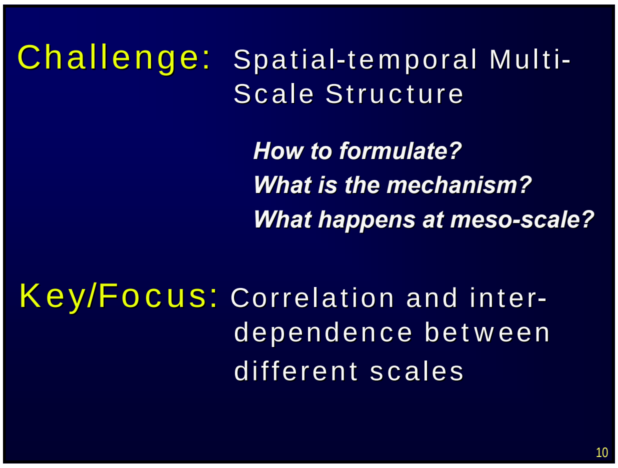
Under the same operating conditions

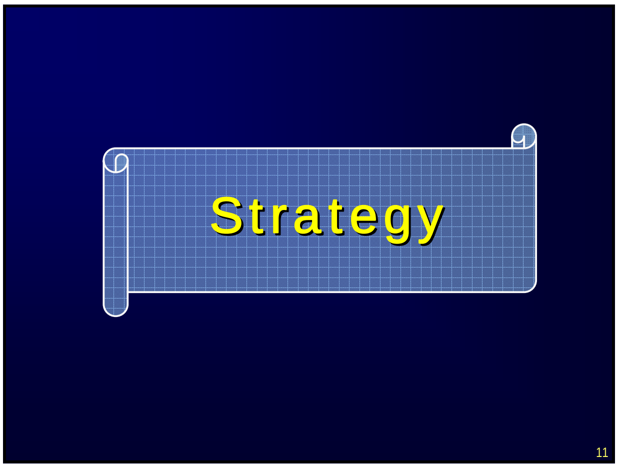
6

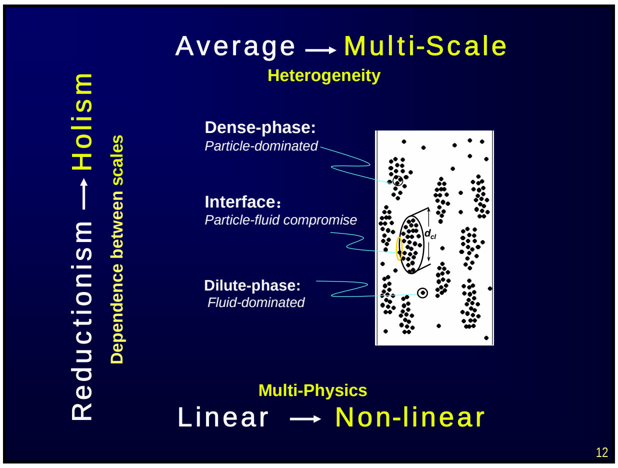

4. Critical influence of structural changes on transport and reaction
C_{do}
Heterogeneity
influence
$C_d = 0.032\ C_{do}$
Orientation
influence
$C_d = 15.4\ C_{do}$
Same
Volume of unit
Number of particles
Gas flow rate
7

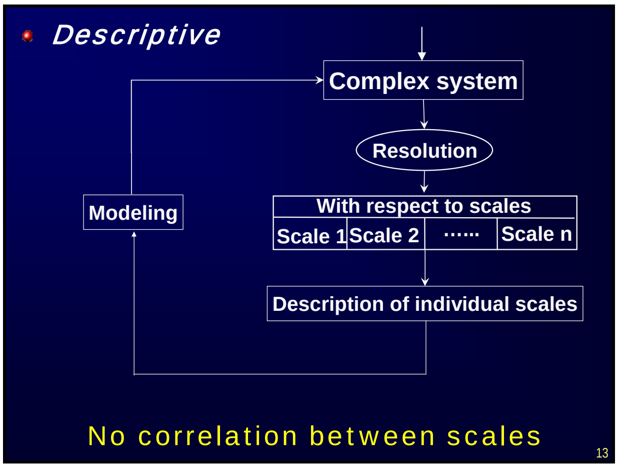

Structural influences on transport properties
—— Meso-scale clusters
$\bar{C}_D$= 18.6
Local
$\bar{C}_D$= 5.43
Local & Radial
$\bar{C}_D$= 2.85
8

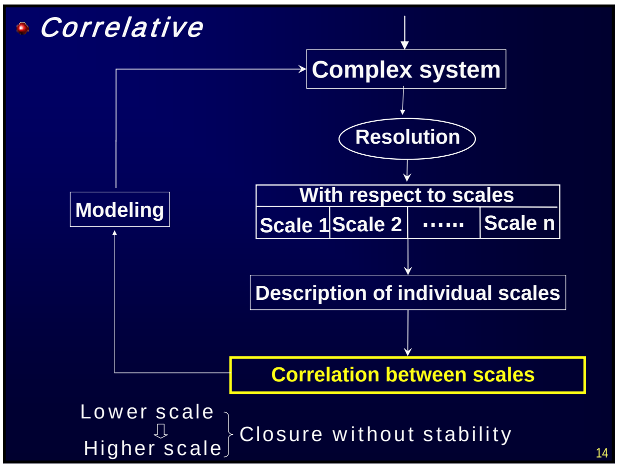

Structural influences on transport properties
—— Drag coefficients in different phases
Dense-phase:
$C_{Dc} \approx 10^5$
Interface:
C_{Di}<10
Dilute-phase:
$C_{Df} \approx 100$
Interdependent
9

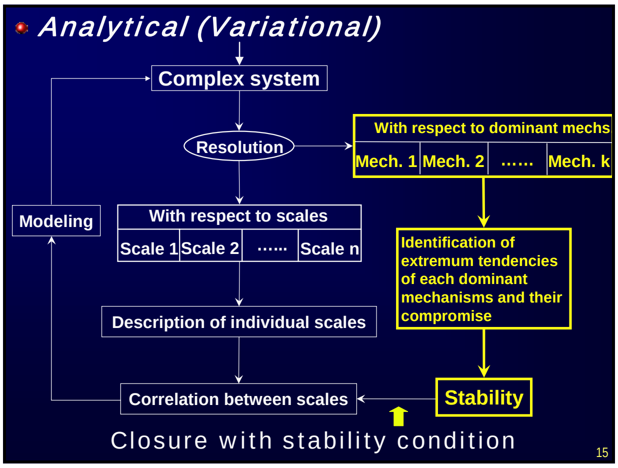

Challenge: Spatial-temporal Multi-Scale Structure
How to formulate?
What is the mechanism?
What happens at meso-scale?
Key/Focus: Correlation and inter-dependence between different scales
10

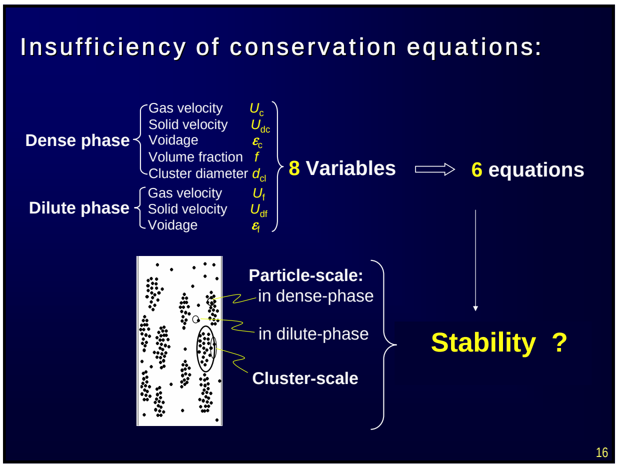

Strategy
11

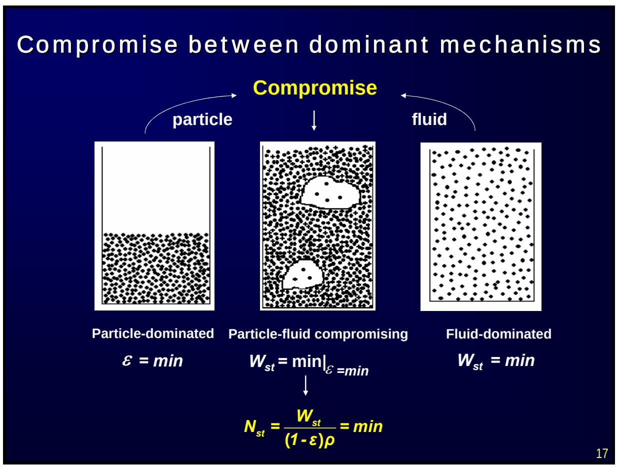

Average → Multi-Scale
Heterogeneity
Dense-phase:
Particle-dominated
Interface:
Particle-fluid compromise
Dilute-phase:
Fluid-dominated
Reductionism → Holism
Dependence between scales
Multi-Physics
Linear → Non-linear
12

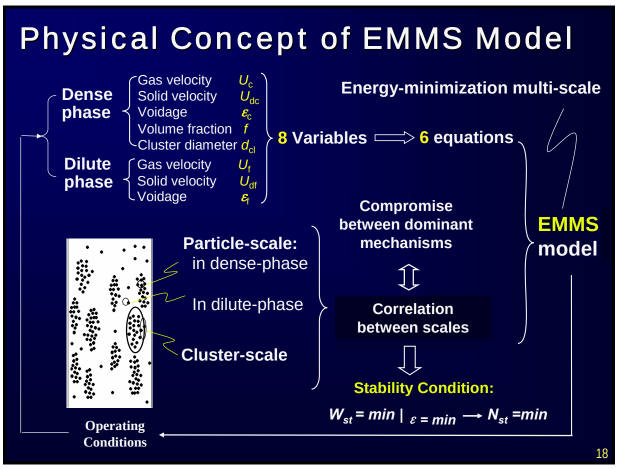

Descriptive
Complex system
Resolution
Modeling
With respect to scales
Scale 1
Scale 2
……
Scale n
Description of individual scales
No correlation between scales
13

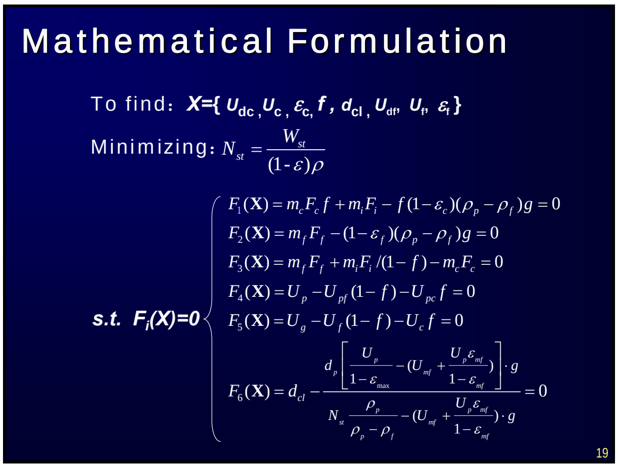

Correlative
Complex system
Resolution
Modeling
With respect to scales
Scale 1
Scale 2
……
Scale n
Description of individual scales
Correlation between scales
Lower scale
Higher scale
Closure without stability
14

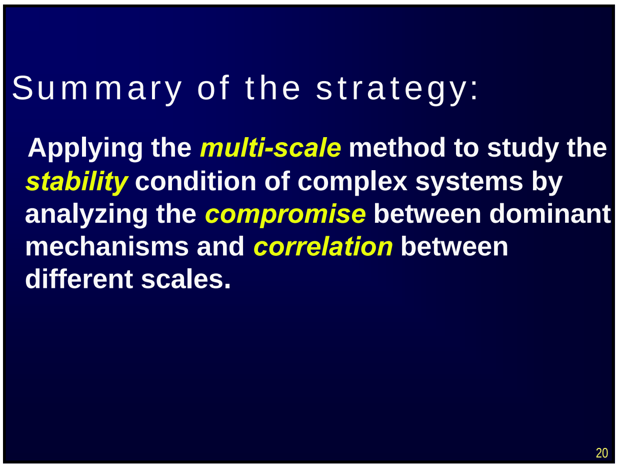

Analytical (Variational)
Complex system
Resolution
With respect to dominant mechs
Mech. 1
Mech. 2
……
Mech. k
Modeling
With respect to scales
Scale 1
Scale 2
……
Scale n
Identification of extremum tendencies of each dominant mechanisms and their compromise
Description of individual scales
Correlation between scales
Stability
Closure with stability condition
15

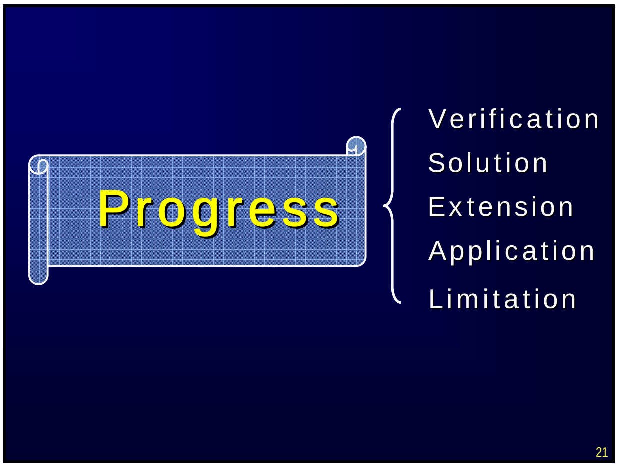

Insufficiency of conservation equations:
Dense phase
Gas velocity U_c
Solid velocity U_{dc}
Voidage ε_c
Volume fraction f
Cluster diameter d_{cl}
Dilute phase
Gas velocity U_f
Solid velocity U_{df}
Voidage ε_f
8 Variables
6 equations
Particle-scale:
in dense-phase
in dilute-phase
Cluster-scale
Stability ?
16

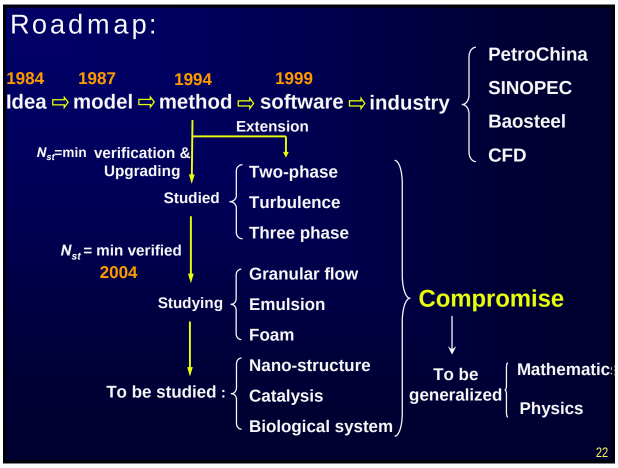

Compromise between dominant mechanisms
Compromise
particle
fluid
Particle-dominated
Particle-fluid compromising
Fluid-dominated
$\varepsilon = min$
$W_{st} = \min|_{\varepsilon = min}$
$W_{st} = min$
$N_{st} = \frac{W_{st}}{(1-\varepsilon)\rho} = min$
17

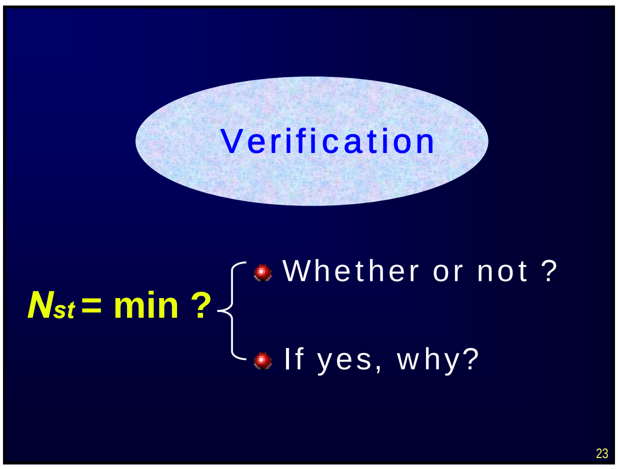

Physical Concept of EMMS Model
Dense phase
Gas velocity U_c
Solid velocity U_{dc}
Voidage ε_c
Volume fraction f
Cluster diameter d_{cl}
Dilute phase
Gas velocity U_f
Solid velocity U_{df}
Voidage ε_f
8 Variables
6 equations
Energy-minimization multi-scale
EMMS model
Particle-scale:
in dense-phase
In dilute-phase
Cluster-scale
Compromise between dominant mechanisms
Correlation between scales
Stability Condition:
$W_{st} = min\,|_{\varepsilon = min} \rightarrow N_{st} = min$
Operating Conditions
18

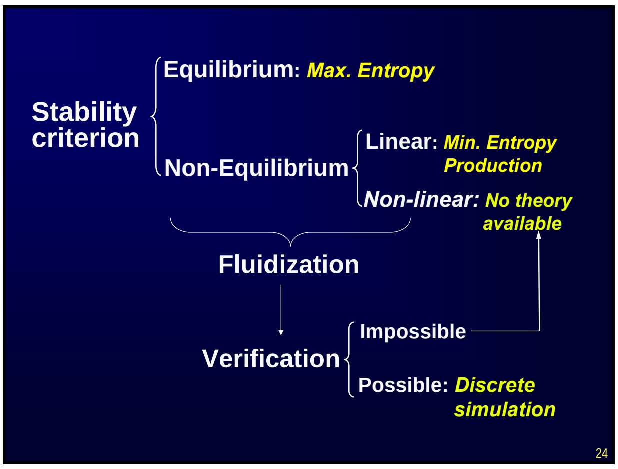

Mathematical Formulation
To find: $X=\{U_{dc}, U_c, \varepsilon_c, f, d_{cl}, U_{df}, U_f, \varepsilon_f\}$
Minimizing: $N_{st} = \frac{W_{st}}{(1-\varepsilon)\rho}$
s.t. $F_i(X)=0$
$F_1(\mathbf{X}) = m_c F_c f + m_i F_i - f(1-\varepsilon_c)(\rho_p - \rho_f)g = 0$
$F_2(\mathbf{X}) = m_f F_f - (1-\varepsilon_f)(\rho_p - \rho_f)g = 0$
$F_3(\mathbf{X}) = m_f F_f + m_i F_i/(1-f) - m_c F_c = 0$
$F_4(\mathbf{X}) = U_p - U_{pf}(1-f) - U_{pc} f = 0$
$F_5(\mathbf{X}) = U_g - U_f(1-f) - U_c f = 0$
$F_6(\mathbf{X}) = d_{cl} - \frac{d_p\left[\frac{U_p}{1-\varepsilon_{max}} - (U_{mf} + \frac{U_p \varepsilon_{mf}}{1-\varepsilon_{mf}})\right]\cdot g}{N_{st}\frac{\rho_p}{\rho_p - \rho_f} - (U_{mf} + \frac{U_p \varepsilon_{mf}}{1-\varepsilon_{mf}})\cdot g} = 0$
19

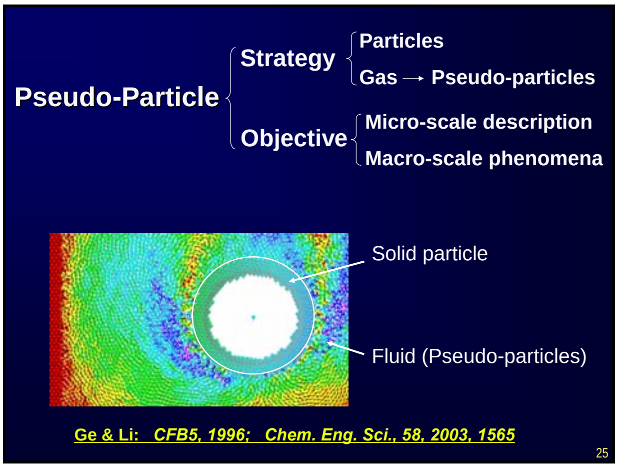

Summary of the strategy:
Applying the multi-scale method to study the stability condition of complex systems by analyzing the compromise between dominant mechanisms and correlation between different scales.
20

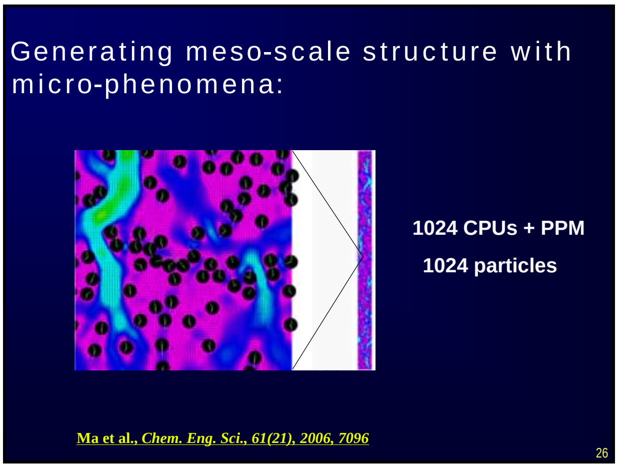

Progress
Verification
Solution
Extension
Application
Limitation
21

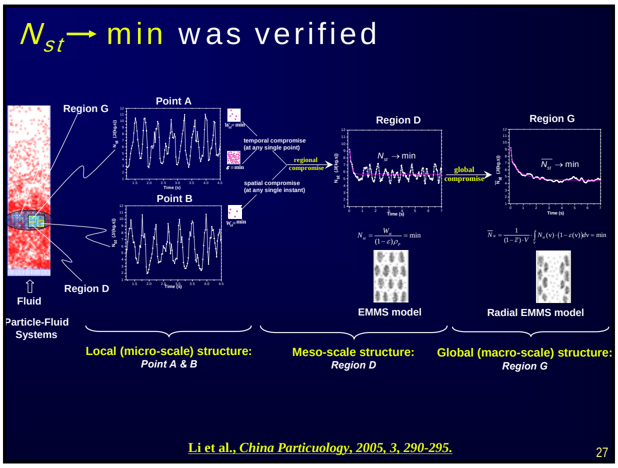

Roadmap:
1984 Idea ⇨ 1987 model ⇨ 1994 method ⇨ 1999 software ⇨ industry
PetroChina
SINOPEC
Baosteel
CFD
Extension
N_{st}=min verification & Upgrading
Studied
Two-phase
Turbulence
Three phase
N_{st}= min verified 2004
Studying
Granular flow
Emulsion
Foam
To be studied :
Nano-structure
Catalysis
Biological system
Compromise
To be generalized
Mathematics
Physics
22

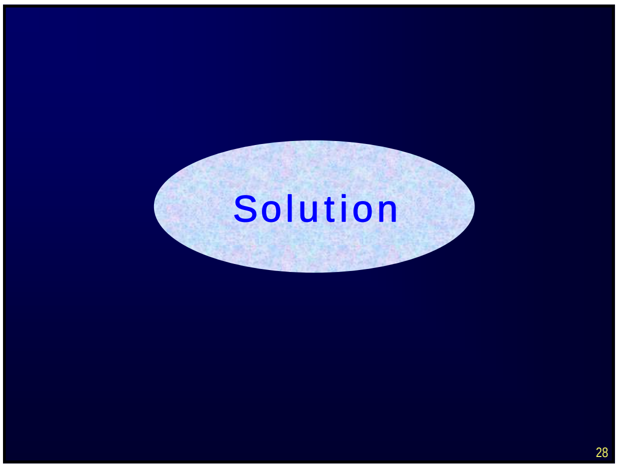

Verification
N_{st}= min ?
Whether or not ?
If yes, why?
23

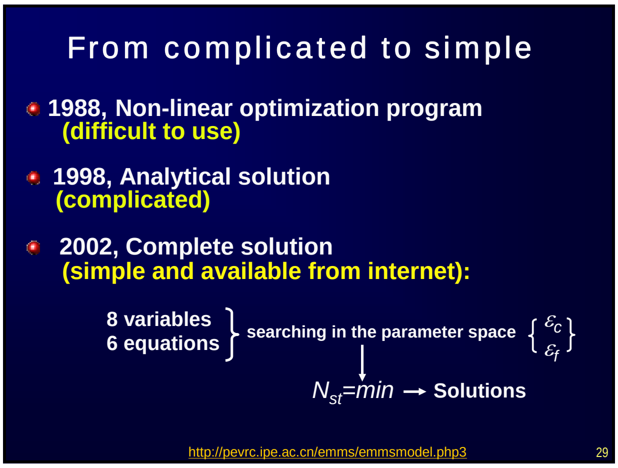

Stability criterion
Equilibrium: Max. Entropy
Non-Equilibrium
Linear: Min. Entropy Production
Non-linear: No theory available
Fluidization
Verification
Impossible
Possible: Discrete simulation
24

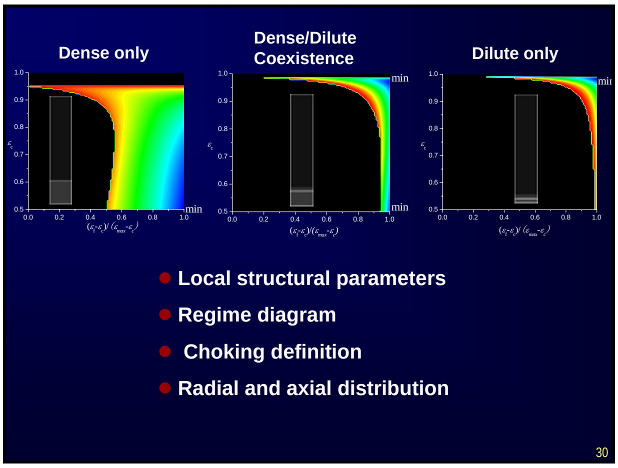

Pseudo-Particle
Strategy
Particles
Gas → Pseudo-particles
Objective
Micro-scale description
Macro-scale phenomena
Solid particle
Fluid (Pseudo-particles)
Ge & Li: CFB5, 1996; Chem. Eng. Sci., 58, 2003, 1565
25

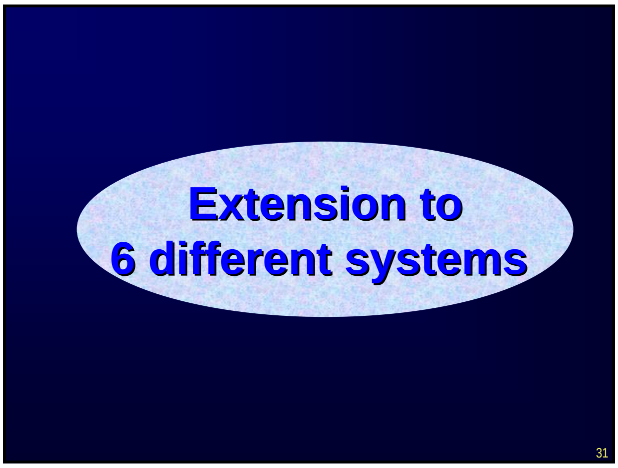

Generating meso-scale structure with micro-phenomena:
1024 CPUs + PPM
1024 particles
Ma et al., Chem. Eng. Sci., 61(21), 2006, 7096
26

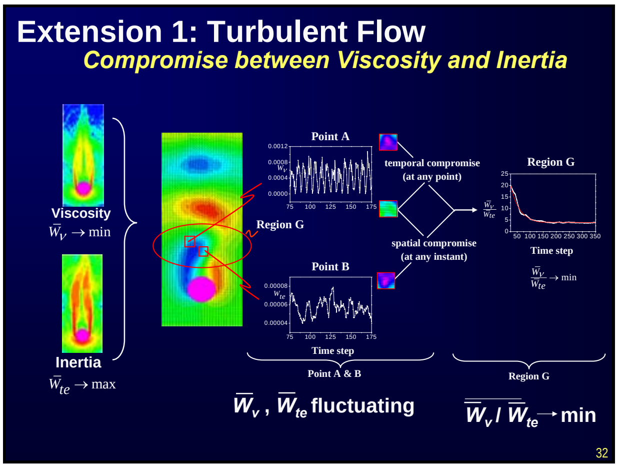

N_{st} → min was verified
Region G
Point A
Point B
Region D
Fluid
Particle-Fluid Systems
temporal compromise
spatial compromise
regional compromise
global compromise
Region D
Region G
EMMS model
Radial EMMS model
Local (micro-scale) structure: Point A & B
Meso-scale structure: Region D
Global (macro-scale) structure: Region G
Li et al., China Particuology, 2005, 3, 290-295.
27

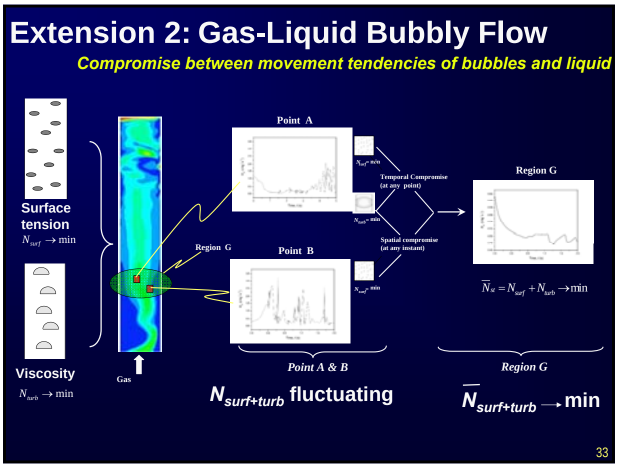

Solution
28

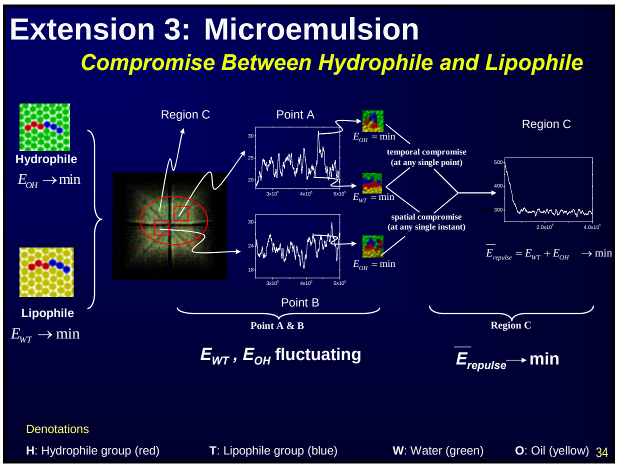

From complicated to simple
1988, Non-linear optimization program (difficult to use)
1998, Analytical solution (complicated)
2002, Complete solution (simple and available from internet):
8 variables
6 equations
searching in the parameter space
ε_c
ε_f
N_{st}=min → Solutions
http://pevrc.ipe.ac.cn/emms/emmsmodel.php3
29

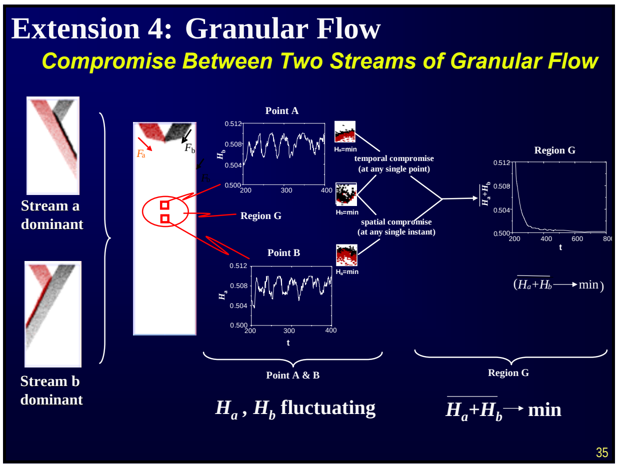

Dense only
Dense/Dilute Coexistence
Dilute only
Local structural parameters
Regime diagram
Choking definition
Radial and axial distribution
30

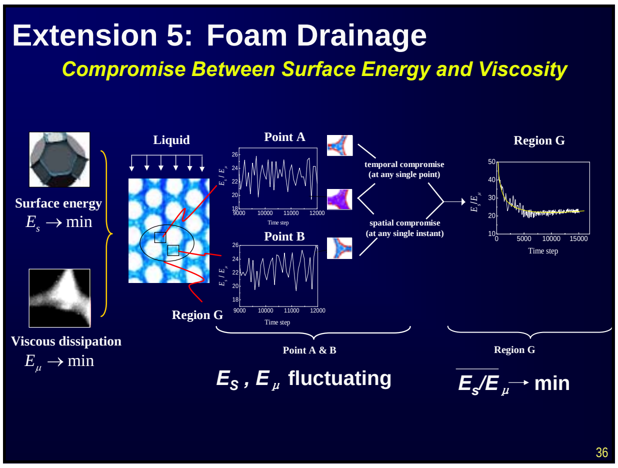

Extension to
6 different systems
31

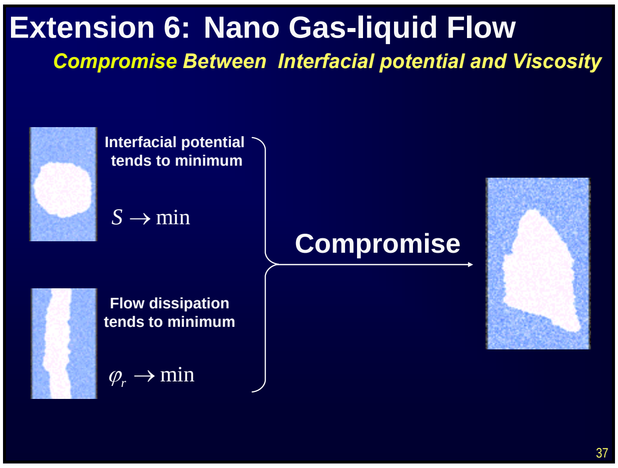

Extension 1: Turbulent Flow
Compromise between Viscosity and Inertia
Viscosity
$\overline{W}_v \to$ min
Inertia
$\overline{W}_{te} \to$ max
Point A
Region G
Point B
temporal compromise (at any point)
spatial compromise (at any instant)
Time step
Point A & B
W_v , W_{te} fluctuating
$\overline{W}_v / \overline{W}_{te} \to$ min
32

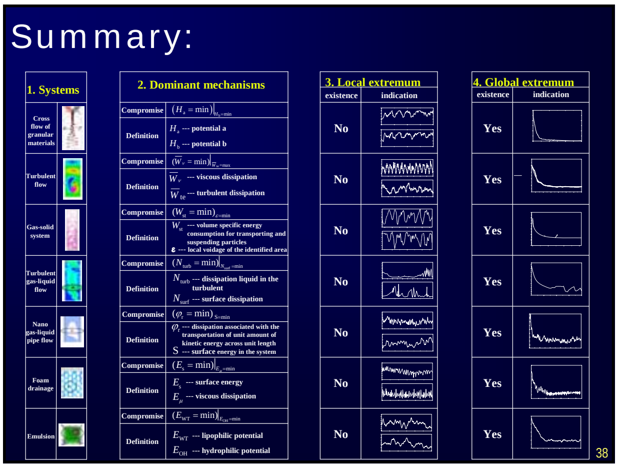

Extension 2: Gas-Liquid Bubbly Flow
Compromise between movement tendencies of bubbles and liquid
Surface tension
$N_{surf} \to$ min
Viscosity
$N_{turb} \to$ min
Gas
Point A
Point B
Region G
Temporal Compromise (at any point)
Spatial compromise (at any instant)
$\overline{N}_{st} = \overline{N}_{surf} + \overline{N}_{turb} \to$ min
Point A & B
$N_{surf+turb}$ fluctuating
$\overline{N}_{surf+turb} \to$ min
33

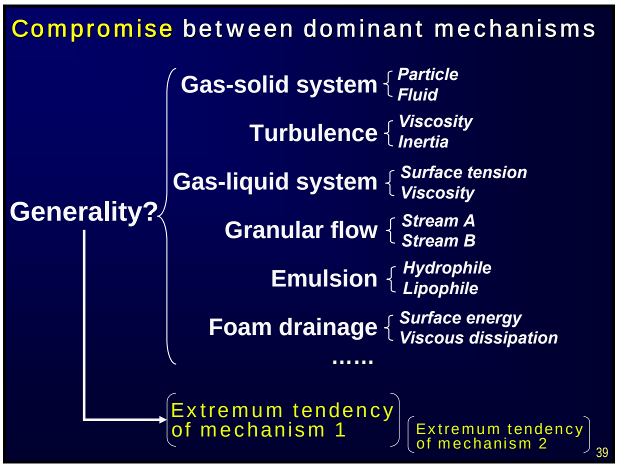

Extension 3: Microemulsion
Compromise Between Hydrophile and Lipophile
Hydrophile
$E_{OH} \to$ min
Lipophile
$E_{WT} \to$ min
Region C
Point A
Point B
temporal compromise (at any single point)
spatial compromise (at any single instant)
$E_{repulse} = E_{WT} + E_{OH} \to$ min
Point A & B
E_{WT} , E_{OH} fluctuating
$\overline{E}_{repulse} \to$ min
Denotations
H: Hydrophile group (red)
T: Lipophile group (blue)
W: Water (green)
O: Oil (yellow)
34

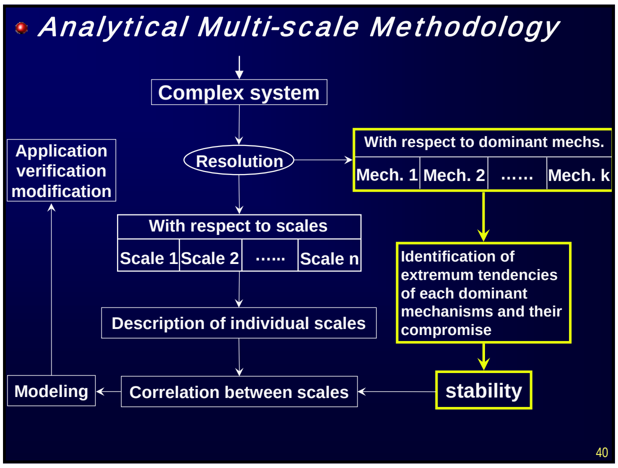

Extension 4: Granular Flow
Compromise Between Two Streams of Granular Flow
Stream a dominant
Stream b dominant
Point A
Point B
Region G
temporal compromise (at any single point)
spatial compromise (at any single instant)
$(\overline{H_a+H_b} \to$ min$)$
Point A & B
H_a , H_b fluctuating
$\overline{H_a+H_b} \to$ min
35

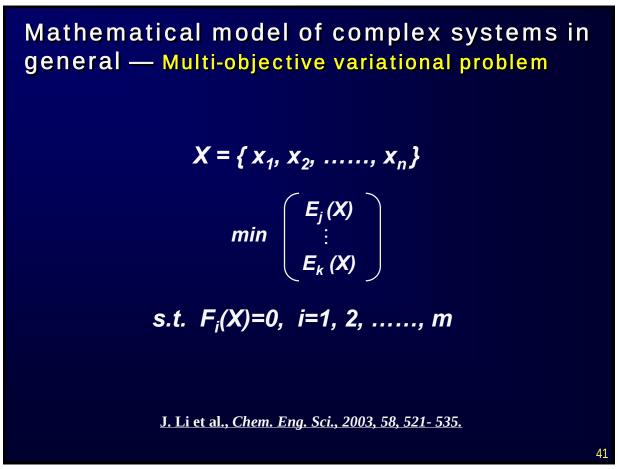

Extension 5: Foam Drainage
Compromise Between Surface Energy and Viscosity
Surface energy
$E_s \to$ min
Viscous dissipation
$E_\mu \to$ min
Liquid
Point A
Point B
Region G
temporal compromise (at any single point)
spatial compromise (at any single instant)
Time step
Point A & B
E_S , E_μ fluctuating
$\overline{E_S / E_\mu} \to$ min
36


Extension 6: Nano Gas-liquid Flow
Compromise Between Interfacial potential and Viscosity
Interfacial potential tends to minimum
S → min
Flow dissipation tends to minimum
φr → min
Compromise
37

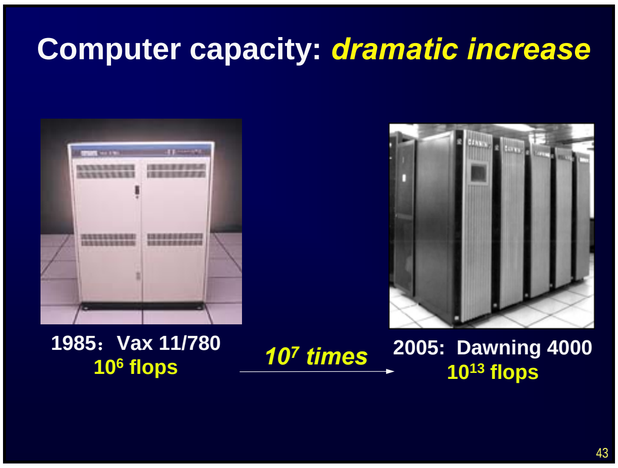

Summary:
1. Systems
2. Dominant mechanisms
3. Local extremum
existence
indication
4. Global extremum
existence
indication
Cross flow of granular materials
Compromise (Ha = min)|Hb=min
Definition Ha --- potential a
Hb --- potential b
No
Yes
Turbulent flow
Compromise (Wv = min)|Wte=max
Definition Wv --- viscous dissipation
Wte --- turbulent dissipation
No
Yes
Gas-solid system
Compromise (Wst = min)ε=min
Definition Wst --- volume specific energy consumption for transporting and suspending particles
ε --- local voidage of the identified area
No
Yes
Turbulent gas-liquid flow
Compromise (Nturb = min)|Nsurf=min
Definition Nturb --- dissipation liquid in the turbulent
Nsurf --- surface dissipation
No
Yes
Nano gas-liquid pipe flow
Compromise (φr = min) S=min
Definition φr --- dissipation associated with the transportation of unit amount of kinetic energy across unit length
S --- surface energy in the system
No
Yes
Foam drainage
Compromise (Es = min)|Eμ=min
Definition Es --- surface energy
Eμ --- viscous dissipation
No
Yes
Emulsion
Compromise (EWT = min)|EOH=min
Definition EWT --- lipophilic potential
EOH --- hydrophilic potential
No
Yes
38

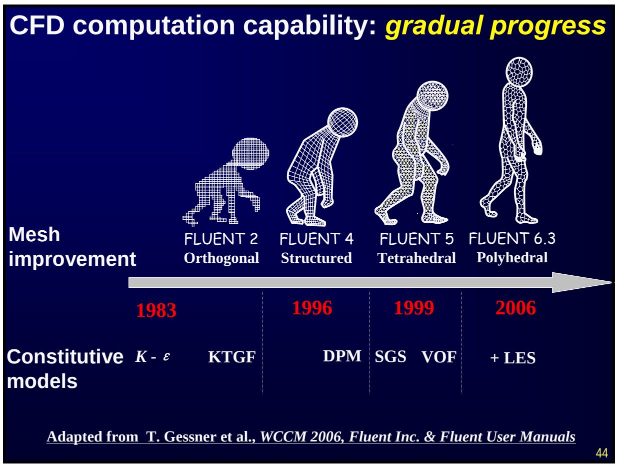

Compromise between dominant mechanisms
Generality?
Gas-solid system { Particle
Fluid
Turbulence { Viscosity
Inertia
Gas-liquid system { Surface tension
Viscosity
Granular flow { Stream A
Stream B
Emulsion { Hydrophile
Lipophile
Foam drainage { Surface energy
Viscous dissipation
……
Extremum tendency of mechanism 1
Extremum tendency of mechanism 2
39

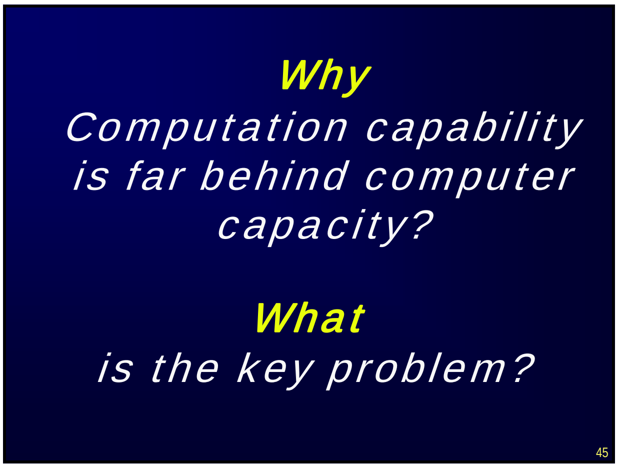

Analytical Multi-scale Methodology
Complex system
Application verification modification
Resolution
With respect to dominant mechs.
Mech. 1
Mech. 2
……
Mech. k
With respect to scales
Scale 1
Scale 2
……
Scale n
Identification of extremum tendencies of each dominant mechanisms and their compromise
Description of individual scales
Modeling
Correlation between scales
stability
40

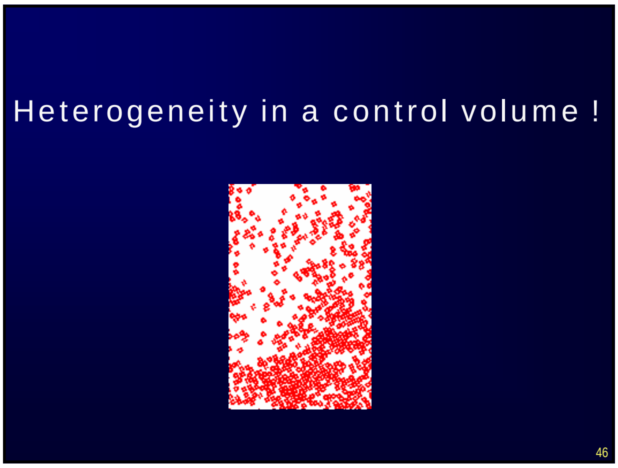

Mathematical model of complex systems in general — Multi-objective variational problem
X = { x1, x2, ……, xn}
min Ej (X) ⋮ Ek (X)
s.t. Fi(X)=0, i=1, 2, ……, m
J. Li et al., Chem. Eng. Sci., 2003, 58, 521- 535.
41

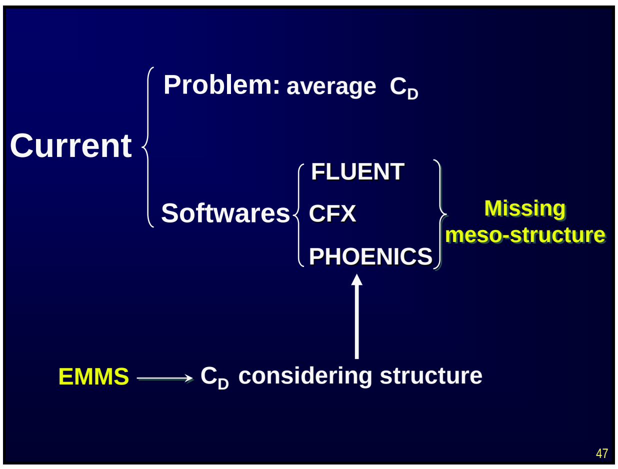

Applications in CFD
42

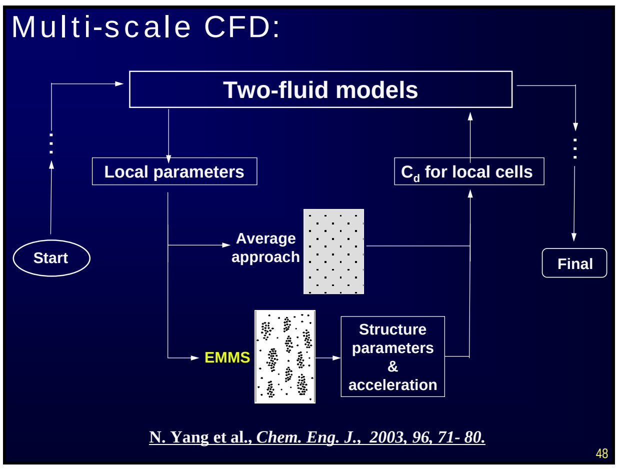

Computer capacity: dramatic increase
1985: Vax 11/780
10^6 flops
10^7 times
2005: Dawning 4000
10^13 flops
43

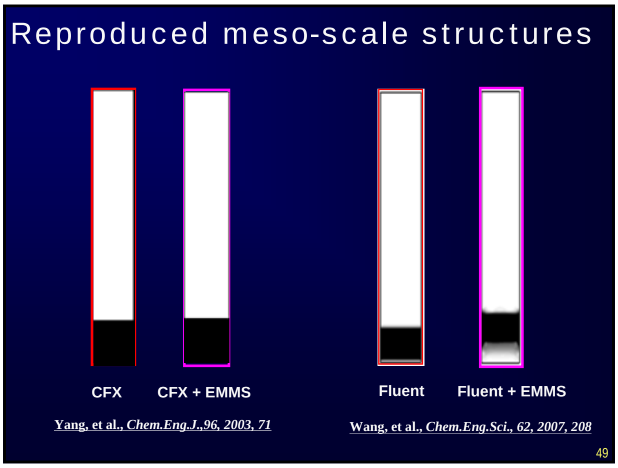

CFD computation capability: gradual progress
Mesh improvement
FLUENT 2 Orthogonal
FLUENT 4 Structured
FLUENT 5 Tetrahedral
FLUENT 6.3 Polyhedral
1983
1996
1999
2006
Constitutive models
K - ε
KTGF
DPM
SGS
VOF
+ LES
Adapted from T. Gessner et al., WCCM 2006, Fluent Inc. & Fluent User Manuals
44

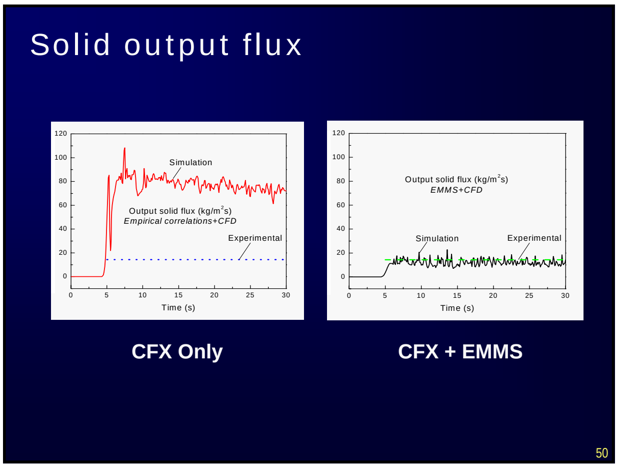

Why
Computation capability is far behind computer capacity?
What
is the key problem?
45

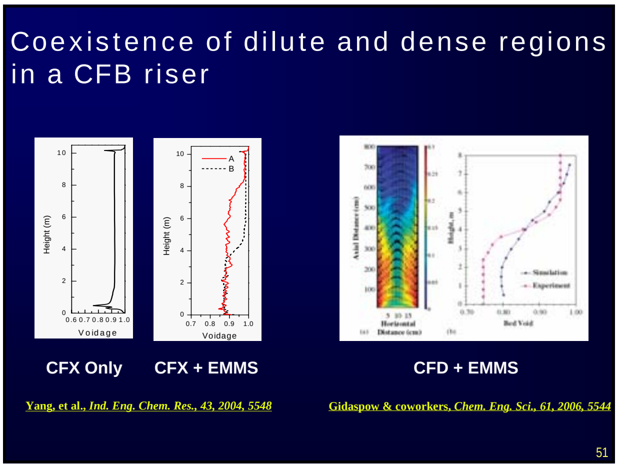

Heterogeneity in a control volume !
46

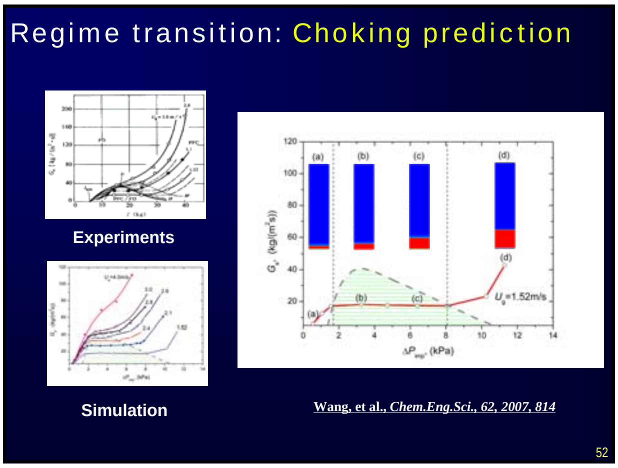

Current
Problem: average C_D
Softwares
FLUENT
CFX
PHOENICS
Missing meso-structure
EMMS
C_D considering structure
47

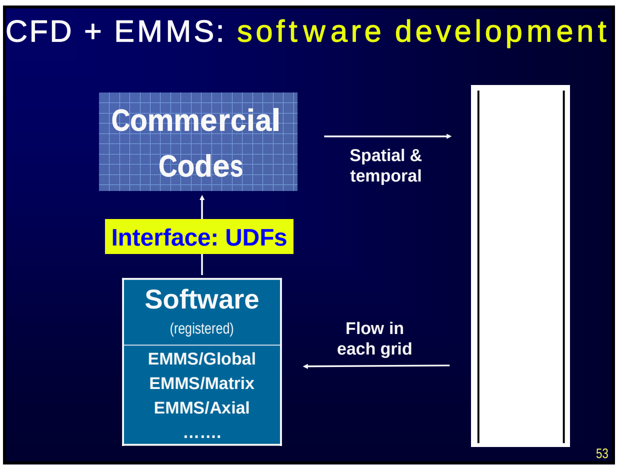

Multi-scale CFD:
Two-fluid models
Local parameters
C_d for local cells
Start
Average approach
Final
EMMS
Structure parameters & acceleration
N. Yang et al., Chem. Eng. J., 2003, 96, 71- 80.
48

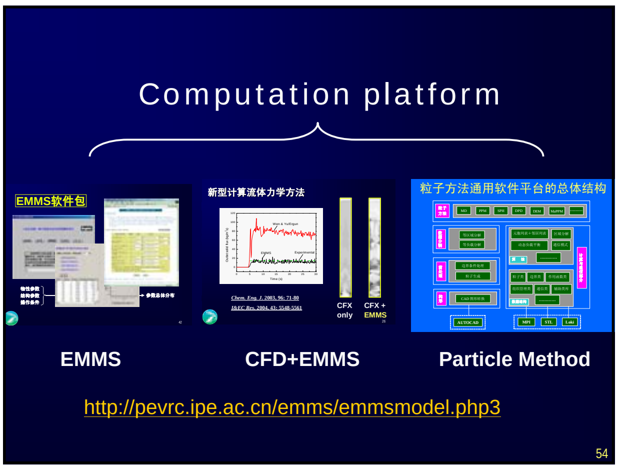

Reproduced meso-scale structures
CFX
CFX + EMMS
Fluent
Fluent + EMMS
Yang, et al., Chem.Eng.J.,96, 2003, 71
Wang, et al., Chem.Eng.Sci., 62, 2007, 208
49

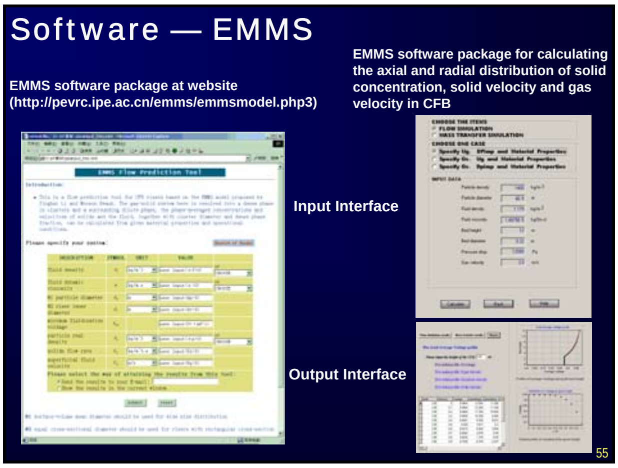

Solid output flux
Simulation
Output solid flux (kg/m²s)
Empirical correlations+CFD
Experimental
Time (s)
Output solid flux (kg/m²s)
EMMS+CFD
Simulation
Experimental
Time (s)
CFX Only
CFX + EMMS
50

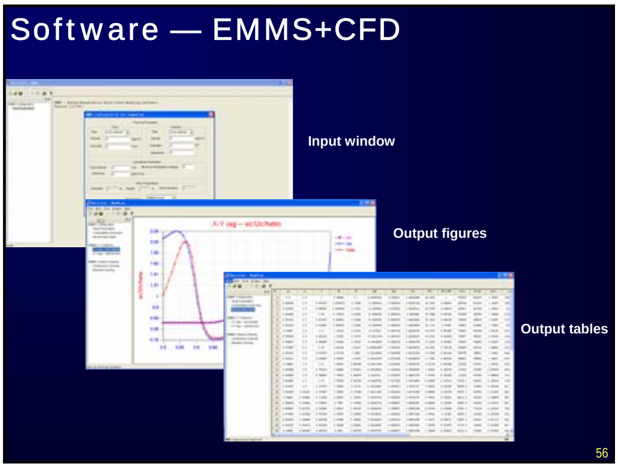

Coexistence of dilute and dense regions in a CFB riser
Height (m)
Voidage
CFX Only
CFX + EMMS
CFD + EMMS
Yang, et al., Ind. Eng. Chem. Res., 43, 2004, 5548
Gidaspow & coworkers, Chem. Eng. Sci., 61, 2006, 5544
51

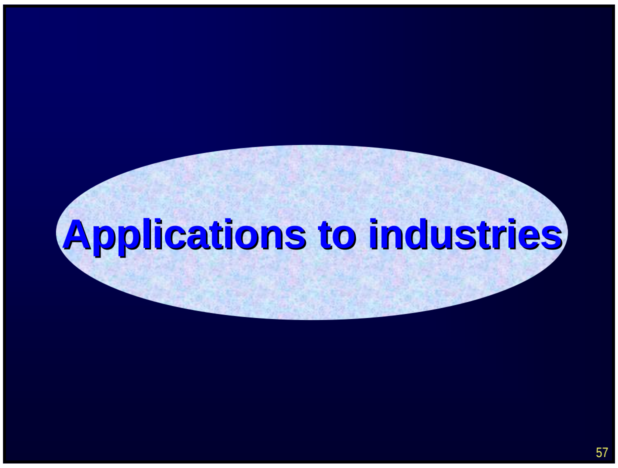

Regime transition: Choking prediction
Experiments
Simulation
Wang, et al., Chem.Eng.Sci., 62, 2007, 814
52

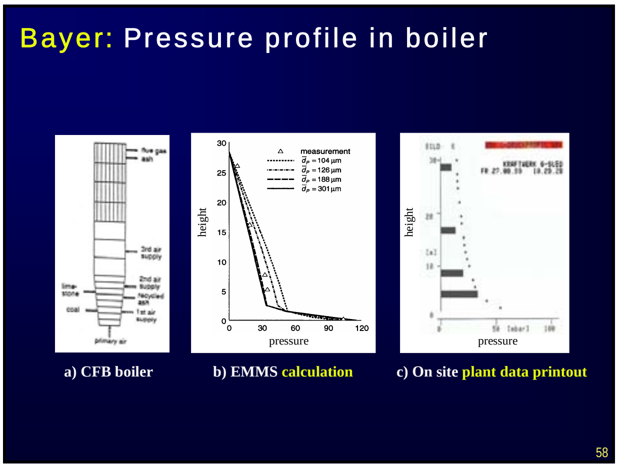

CFD + EMMS: software development
Commercial Codes
Interface: UDFs
Software
(registered)
EMMS/Global
EMMS/Matrix
EMMS/Axial
…….
Spatial & temporal
Flow in each grid
53

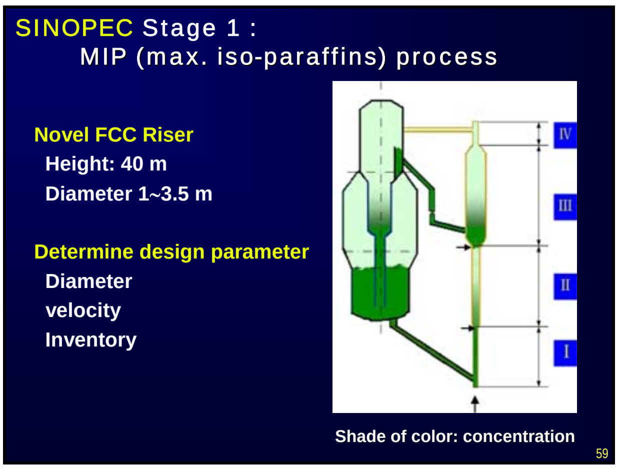

Computation platform
EMMS软件包
新型计算流体力学方法
粒子方法通用软件平台的总体结构
EMMS
CFD+EMMS
Particle Method
http://pevrc.ipe.ac.cn/emms/emmsmodel.php3
54

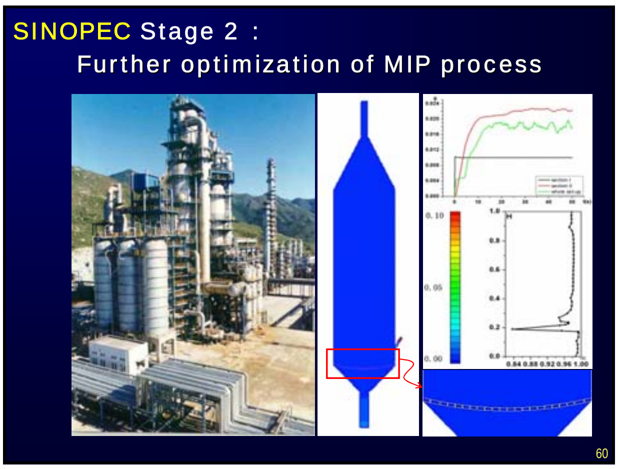

Software — EMMS
EMMS software package at website
(http://pevrc.ipe.ac.cn/emms/emmsmodel.php3)
EMMS software package for calculating the axial and radial distribution of solid concentration, solid velocity and gas velocity in CFB
Input Interface
Output Interface
55

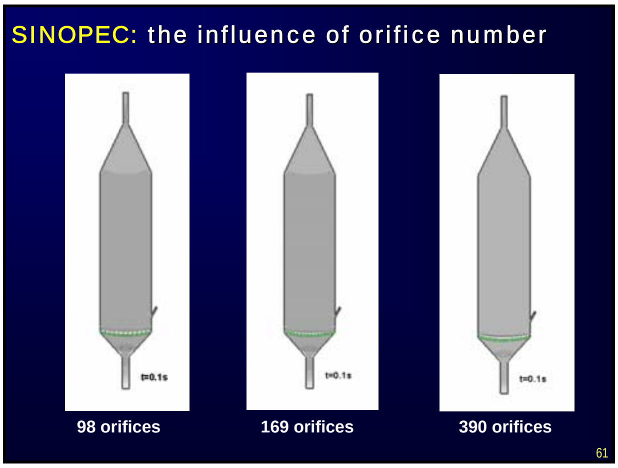

Software — EMMS+CFD
Input window
Output figures
Output tables
56

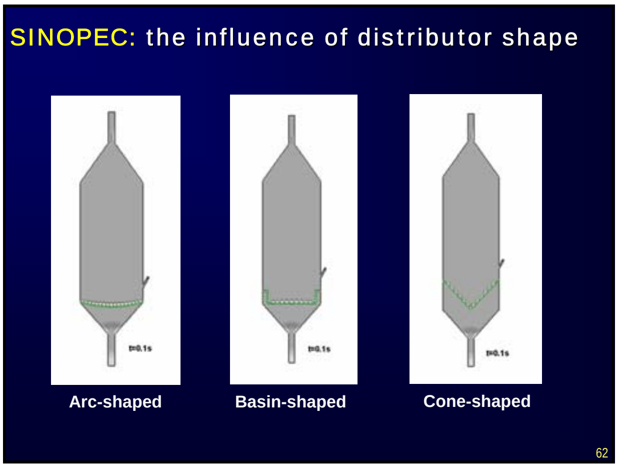

Applications to industries
57

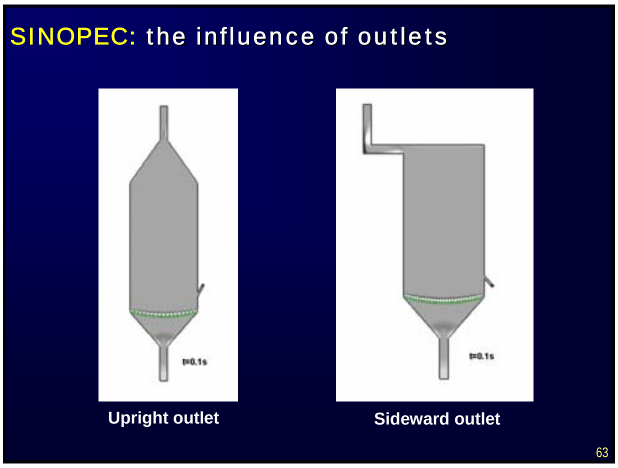

Bayer: Pressure profile in boiler
height
pressure
a) CFB boiler
b) EMMS calculation
c) On site plant data printout
58

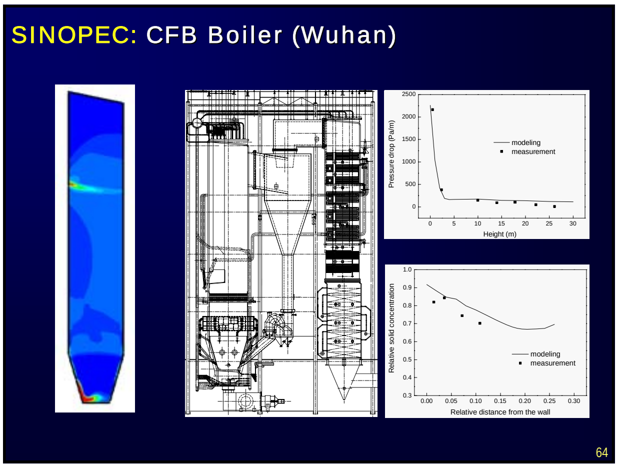

SINOPEC Stage 1 :
MIP (max. iso-paraffins) process
Novel FCC Riser
Height: 40 m
Diameter 1~3.5 m
Determine design parameter
Diameter
velocity
Inventory
IV
III
II
I
Shade of color: concentration
59

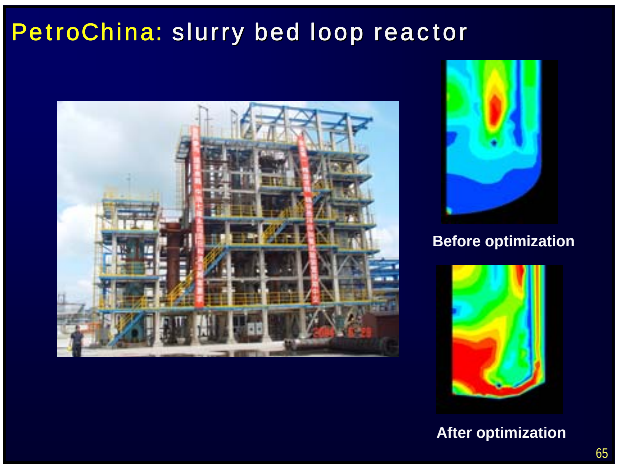

SINOPEC Stage 2 :
Further optimization of MIP process
60

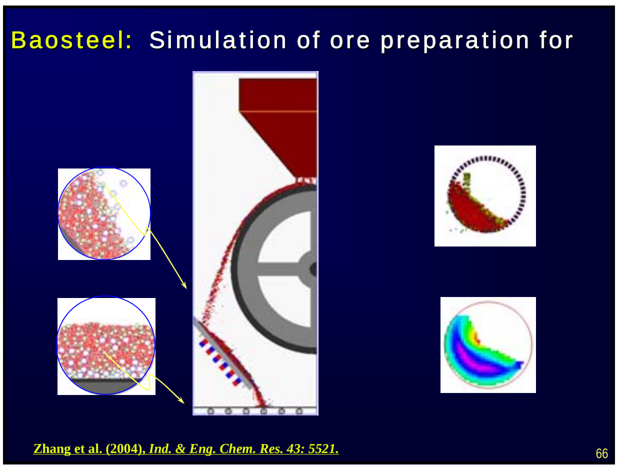

SINOPEC: the influence of orifice number
t=0.1s
t=0.1s
t=0.1s
98 orifices
169 orifices
390 orifices
61

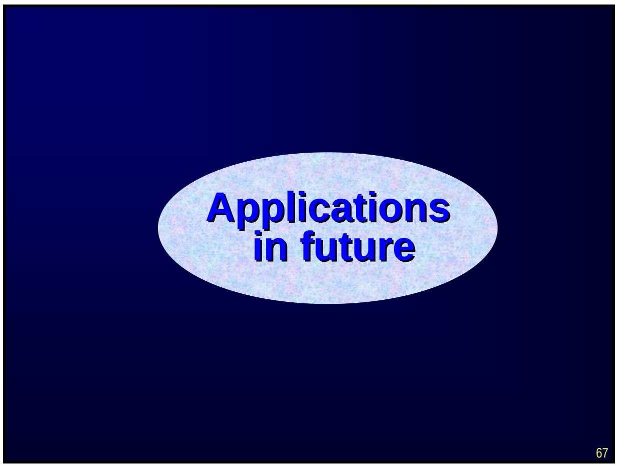

SINOPEC: the influence of distributor shape
t=0.1s
t=0.1s
t=0.1s
Arc-shaped
Basin-shaped
Cone-shaped
62

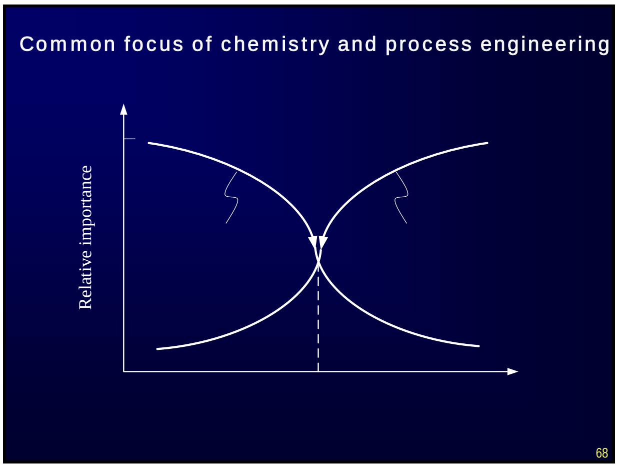

SINOPEC: the influence of outlets
t=0.1s
t=0.1s
Upright outlet
Sideward outlet
63

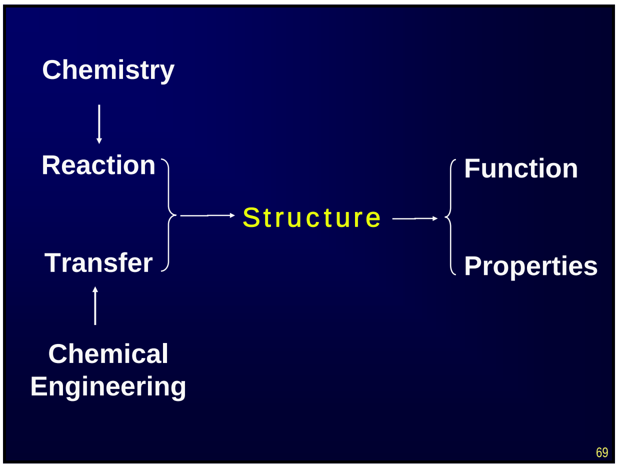

SINOPEC: CFB Boiler (Wuhan)
Pressure drop (Pa/m)
modeling
measurement
Height (m)
Relative solid concentration
modeling
measurement
Relative distance from the wall
64

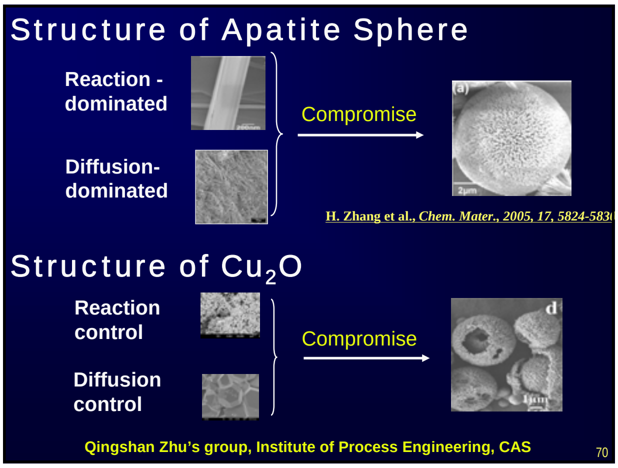

PetroChina: slurry bed loop reactor
Before optimization
After optimization
65

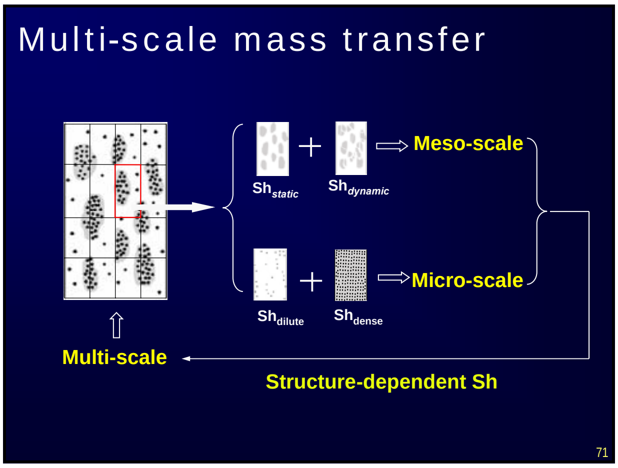

Baosteel: Simulation of ore preparation for
Zhang et al. (2004), Ind. & Eng. Chem. Res. 43: 5521.
66

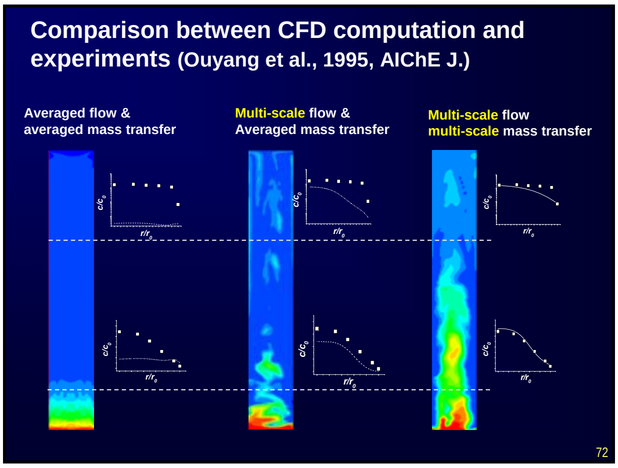

Applications
in future
67


Common focus of chemistry and process engineering
Relative importance
68

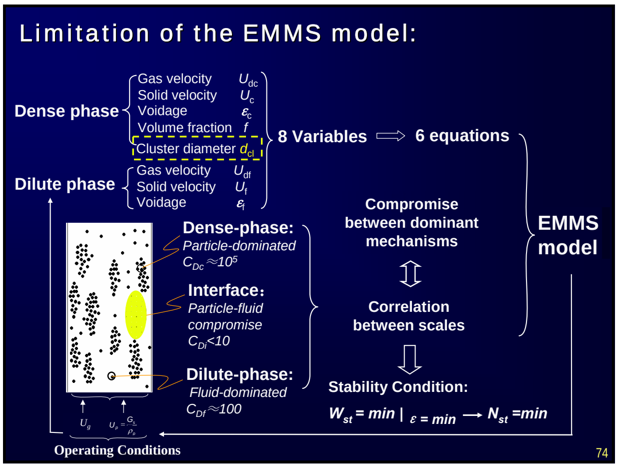

Chemistry
Reaction
Transfer
Chemical
Engineering
Structure
Function
Properties
69

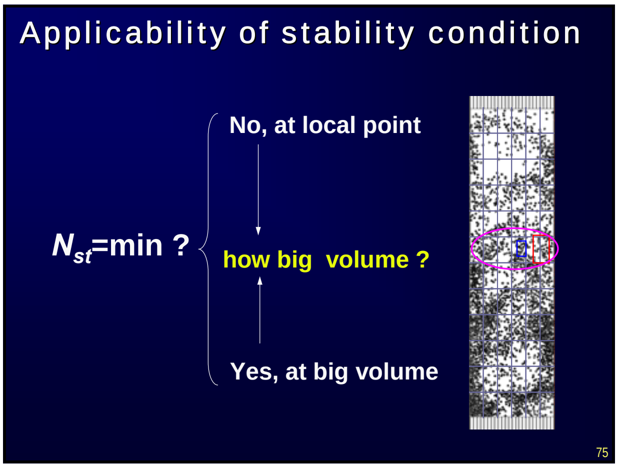

Structure of Apatite Sphere
Reaction -
dominated
Diffusion-
dominated
Compromise
H. Zhang et al., Chem. Mater., 2005, 17, 5824-583
Structure of Cu_2O
Reaction
control
Diffusion
control
Compromise
Qingshan Zhu's group, Institute of Process Engineering, CAS
70

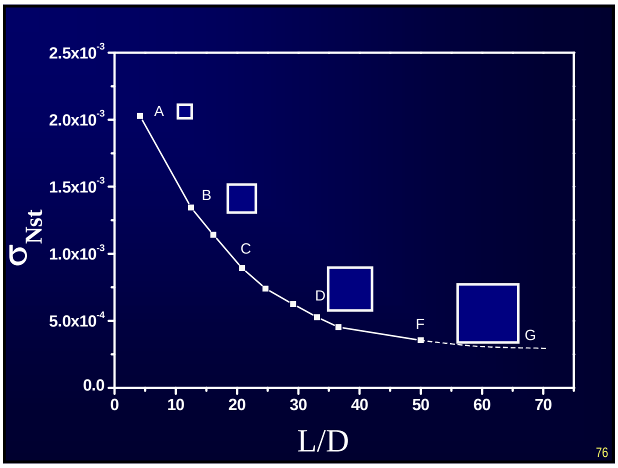

Multi-scale mass transfer
Sh_{static}
$Sh_{dynamic}$
Meso-scale
Sh_{dilute}
Sh_{dense}
Micro-scale
Multi-scale
Structure-dependent Sh
71

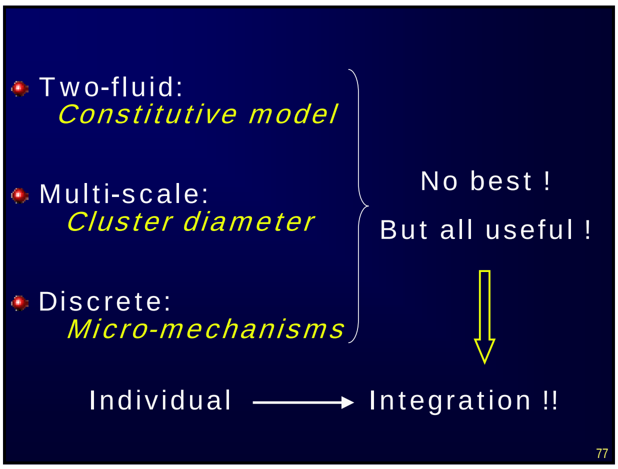

Comparison between CFD computation and
experiments (Ouyang et al., 1995, AIChE J.)
Averaged flow &
averaged mass transfer
Multi-scale flow &
Averaged mass transfer
Multi-scale flow
multi-scale mass transfer
72

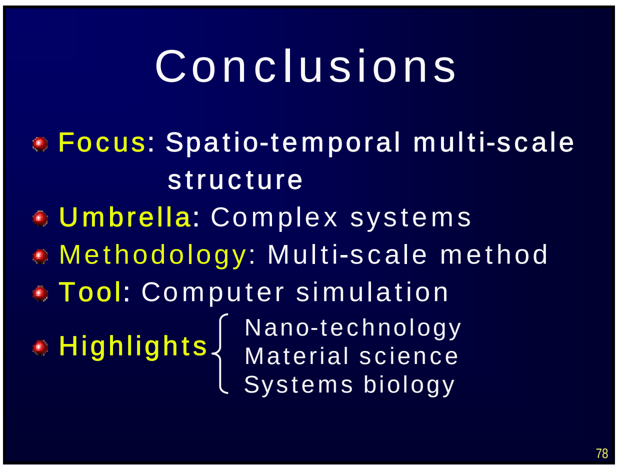

Limitations & Difficulties
73


Limitation of the EMMS model:
Dense phase
Gas velocity U_{dc}
Solid velocity U_c
Voidage ε_c
Volume fraction f
Cluster diameter d_{cl}
Dilute phase
Gas velocity U_{df}
Solid velocity U_f
Voidage ε_f
8 Variables
6 equations
Dense-phase:
Particle-dominated
$C_{Dc} \approx 10^5$
Interface:
Particle-fluid compromise
$C_{Di} < 10$
Dilute-phase:
Fluid-dominated
$C_{Df} \approx 100$
Compromise between dominant mechanisms
Correlation between scales
EMMS model
Stability Condition:
$W_{st} = min \mid_{\varepsilon = min} \rightarrow N_{st} = min$
Operating Conditions
74


Applicability of stability condition
N_{st}=min ?
No, at local point
how big volume ?
Yes, at big volume
75


2.5x10-3
2.0x10-3
1.5x10-3
1.0x10-3
5.0x10-4
0.0
σ_{Nst}
A
B
C
D
F
G
0
10
20
30
40
50
60
70
L/D
76


Two-fluid:
Constitutive model
Multi-scale:
Cluster diameter
Discrete:
Micro-mechanisms
No best !
But all useful !
Individual
Integration !!
77


Conclusions
Focus: Spatio-temporal multi-scale structure
Umbrella: Complex systems
Methodology: Multi-scale method
Tool: Computer simulation
Highlights
Nano-technology
Material science
Systems biology
78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ETH (Swiss Federal Institute of Technology)
AvH (Alexander von Humboldt Foundation)
79


Thank you !
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