Mesosciences: Enabling Realtime Simulation of Chemical Engineering

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Current Challenges

Three Mesoscales & Two Gaps

Focusing on Mesoscales

Compromise in Competition

Realizing Virtual Reality

Exploring Realtime Simulation

Exploring Mesoscience

An Transdisciplinary Science
Current Challenges

Three Mesoscales & Two Gaps
All industries related to physical and chemical processing of materials and energies

Increasing Generality:

Transport phenomena & Reaction engineering

Increasing Understanding:

A new age

Virtual reality
Material design
Process quantification
System optimization

Meso

Filtration
Separation
Evaporation
Condensation
Absorption
Distillation
Extraction
Drying

Chemical Reaction

Transfer
Mass
Energy
Momentum

Common Principle

Global Analysis

Radial & Axial Distribution

Unit operation

1920s

1950s

Multilevel and Multiscale Nature

Material and interfacial structure
Mesoscale 1

Heterogeneous flow structure
Mesoscale 2

Integration of units
Mesoscale 3

Bottlenecks for three levels

Boundary scales

Multi-level

Material

Molecule /Atom → Assembly → Particle → Aggregate → Unit operation

Reactors

System

Environment

From Molecule

Direct Scale-up → Virtual Process Engineering

To Market

Similar features in life systems

**Multi-scale**
- Amino acid
- Secondary structure
- Protein
- Macrobiomolecule complex
- Cell
- Tissue
- Organ

**Meso-scale 1**
- Macrobiomolecule

**Meso-scale 2**
- Cell

**Meso-scale 3**
- Life

Li J. et al., *Particuology*, 2010, 8(6): 634-639
**Complexity: Multiscale Structure**

**Material:**
- Hydroxyapatite: $Ca_5(OH)(PO_4)_3$

**Reactor:**
- Flow, mass transfer, and reaction around a particle
- Affect transport
- $CD = 18.6$
- $CD = 5.43$

**Macro**
- Axial and radial distribution

**Meso?**
Dependence of transport behavior on mesoscale structure

**Without structure**

$C_D = 18.6$

**With only local structure**

$C_D = 5.43$

**With both local and global structure**

$C_D = 2.85$

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Critical influence of mesoscale structures on mass transfer!

Distortion of Real Mechanisms:

**Actual**
Multiscale structure

- **Dilute phase**
  - *Fluid-dominated*
  - $C_D \sim 10^2$
- **Dense phase**
  - *Particle-dominated*
  - $10^5 < C_D < 10^6$
- **Interface**
  - *Particle-Fluid compromise*
  - $1 < C_D < 10^2$

**Averaging Approach**
Uniform structure

- Distorted value
  - $C_D = ?$

---

C

D

\[ ? \]
Definition of Mesoscales

- Relative
- Intermediate

Not only mesoscopic!

- Meso

Mesoscale

Element scale → System scale
Two Gaps between Three Mesoscales

**From Molecules**

- Reaction
- Transport

**Bottlenecks to be overcome**

**Mesoscale 1**

Gap 1 at Particle scale:
Coupling hydrodynamics, transport and reaction

**Mesoscale 2**

- Hydrodynamics
- Transport performance

Gap 2 at Reactor scale:
Coupling physical processes and chemical processes and environment & economic factors

**Mesoscale 3**

- Physical & chemical processes
- Environmental & economic factors

**To Market**

Gaps to be Removed

Focusing on Mesoscales

Compromise in Competition
Multiscale methods: "Meso" is the key

Complex system

Correlative → Variational

Resolution

Modeling → Scale 1 (Scale 2) (Scale 3)

Mech. 1 → Mech. 2 → ..... → Mech. k

Compromise in competition

(Extremum 1) (Extremum 2)

Mesoscale stability

Potential of Mesoscience

Correlation between scales

Meso-scale

Coarse-grained modeling

Modeling 1 → Modeling 2 → Modeling 3

Multiscale methods: Correlative and Variational
Mesoscale Modeling:  

\[ \text{Energy Minimization Multi-Scale (EMMS)} \]

**Resolution Structure**

- Particle scale: \( \epsilon_c U_c U_{pc} \)
  - Dense phase
- Meso-scale: \( f d_{cl} \)
- Global scale: \( U_g U_p \)
  - \( \epsilon \)

**The EMMS Model**

- Meso-stability condition
- Conservation equations

**Resolution dominant mechanisms**

- Particle dominated
  - \( \epsilon = \min \)
  - \( W_{st} = \min \)
- Gas dominated

**Compromise**

\[ W_{st} = \min | \epsilon = \min \]

\[ N_{st} = \frac{W_{st}}{(1 - \epsilon) \rho_p} = \min \]
EMMS Model

Continuity:
\[ fU_{gc} + (1 - f)U_{gf} = U_g \]
\[ fU_{sc} + (1 - f)U_{sf} = U_s \]

Momentum:
\[ fF_{dc} + F_{di} + f \varepsilon _{sc} (\rho_s - \rho_g) g = 0 \]
\[ F_{df} + \varepsilon _{sf} (\rho_s - \rho_g) g = 0 \]

Pressure:
\[ F_{df} + \frac{F_{di}}{1 - f} = F_{dc} \]

Cluster:
\[ d_{cl} = \frac{d_p [U_s / (1 - \varepsilon_{max}) - (U_{mf} + \varepsilon_{mf} U_s / (1 - \varepsilon_{mf}))]}{N_{st} \rho_s / (\rho_s - \rho_g) - (U_{mf} + \varepsilon_{mf} U_s / (1 - \varepsilon_{mf}))} \cdot g \]

Stability condition:
\[ N_{st} = \frac{\rho_g - \rho_s}{\rho_s} \left[ U_g - \frac{\varepsilon_{s} - \varepsilon_{ir}}{1 - \varepsilon_{s}} f (1 - f) U_{gf} \right] \cdot g \rightarrow \min \]

Multi-objective Variational Problem

\[ X = \{ x_1, x_2, \ldots, x_n \} \]

\[ \min \left( \begin{align*} 
E_j (X) \\
\vdots \\
E_k (X) 
\end{align*} \right) \]

s.t. \( F_i (X) = 0, i=1,2, \ldots, m \)
Advantage of EMMS: *Good predictability*

Traditional CFD

EMMS + CFD
**Advantage of EMMS: Extended scalability**

- **Solid Volume Fraction**
- **Height (m):**
  - 7.6m
  - 6.5m
  - 4m
  - 2m
  - 0.72m

**Equations:**

- $U_g = 3.5 \text{ m/s}$
- $H_{init} = 1.70 \text{ m}$
Predictability + Scalability → Industrial application

CFB Boiler  H:36.5 m, L:15.3 m, W:7.22 m
Discrete simulation: Verifying $N_{st}=\min$

\( N_{st} \rightarrow \text{min} \) was verified, but no at microscale
Extension of EMMS: *gas-liquid system*

- **Micro scale:** $\sigma, \mu_l, \rho_l, \rho_g$
- **Meso-scale:** $f_i, d_i, U_{g,i}$
- **Macro scale:** $U_g, U_l$

- **Resolution Structure**
- **Meso-scale Model**
- **Conservation equations + Meso-stability condition**
- **Resolve dominant mechanisms**

Liquid dominated

- $N_{surf} = \text{min}$

Gas dominated

- $N_{turb} = \text{min}$

Compromise

- $N_{turb} = \text{min}$
- $N_{surf} = \text{min}$
Prediction of regime transition


![Graph showing comparison between mesoscale and average models for gas holdup as a function of superficial gas velocity.](image)
Extension of EMMS: *Turbulence model*

Micro scale: $W_v = \text{max}_v$, $W_{te} = \text{min}_e$, $\mu$, $\mu_e$, $\sigma$, $\rho$, $\rho_e$

Meso scale: $f$, $d_e$, $\mu_{le}$, $\mu_{me}$, $\sigma$

Macro scale: $\rho$, $\rho_e$, $\mu$, $\mu_e$, $\sigma$

Resolution dominant mechanisms

- Viscosity dominated
- Inertia dominated

Conservation equations + Meso-stability condition

Compromise

$W_v = \text{min}_v$, $W_{te} = \text{max}_e$
Numerical verification

Simulation with EMMS turbulence model

Turbulent Flow: Compromise between \( \text{Viscosity} \) and \( \text{Inertia} \)

- **Viscosity** \( \bar{W}_v \rightarrow \text{min} \)
- **Inertia** \( \bar{W}_{te} \rightarrow \text{max} \)

\( \bar{W}_v, \bar{W}_{te} \) fluctuating

\( \bar{W}_v / \bar{W}_{te} \rightarrow \text{min} \)
Interaction between two granular flows

A-dominated

\[ H_A = \text{min} \]

A-B compromise

\[ H_A = \text{min} \quad | \quad H_B = \text{min} \]

B-dominated

\[ H_B = \text{min} \]
Granular Flow: *Compromise between* Stream a, Stream b

Stream a dominant

Stream b dominant

$H_a, H_b$ fluctuating

$\overline{H_a + H_b} \rightarrow \min$
Flow induced protein folding

Mechanism A: *Free energy*

Free energy dominate

Mechanism B: *Flow*

Flow dominate

Compromise between the two mechanisms

PMF of flow induced β-switch folding

Han et al. *Biophys. Chem.*, 2015, accepted.
Dynamic Change of Protein Structures

Compromise in competition between dominant mechanisms

\[ X = \{ x_1, x_2, \ldots, x_n \} \]

\[ \min \begin{cases} E_j(X) \\ \vdots \\ E_k(X) \end{cases} \]

s.t. \( F_i(X) = 0, \ i = 1, 2, \ldots, m \)

Physical Principle:
Compromise in competition

Mathematical Formulation:
Multi-objective variational

Exploring Virtual Reality

The EMMS Paradigm
Complex systems (Problem)

\[ X = \{ x_1, x_2, \ldots, x_n \} \]

\[
\begin{align*}
\min \quad & \begin{cases} 
E_j(X) \\
n \quad \vdots \\
E_k(X)
\end{cases} \\
\text{s.t.} \quad & F_i(X) = 0, \quad i = 1, 2, \ldots, m
\end{align*}
\]

Multi-objective variational problem (Modeling)

Software

Computer

The EMMS Paradigm

Structural consistency
Consistency

Structure

Logic

Problem

System

Mesoscale (Cell)

Element

Model → Software → Hardware

System stability

Computation Storage

Communication

Structure stability

Computation Storage

Communication

Elemental interaction

Computation Storage

xPU?
Integration of CPUs and GPUs

**EMMS** → **CPU**

**Macro**

**Meso**

**Micro**: Pseudo-particle → **GPU**

- Interaction
- Information
- Correlation

**Similarity**

- Computation
- Storage
- Communication

1 Petaflops, IPE, CAS
Simulation of rotating drum

3.5x1.5 meter, 9.6 million particles

Real time simulation
Simulation of H1N1 Influenza Virion

(300 million atoms, 2237 proteins, simulated by 1728 GPUs)

Atom simulation of Crystalline Silicon

Petaflops application

Si Nano wire

52nm × 54nm × 0.78 mm
110 billion atoms

CPU
Surface 165Tflops

GPU
Bulk 1.87Pflops

Tianhe-1A, 7168 GPU

Supporting Process Design and Optimization:
Optimization of ore segregator
Coal gasifier optimization
CFB Boiler
Metallurgical Process
Hydrodynamics and reaction in Boiler of Power plant

Industrial applications:
- Multiple-section Reactor
  - 1.4 Mt/a FCC
  - Clean gasoline production
Baosteel Blast Furnace Simulation

- Particle number: $\sim 10^8$
- Particle diameter ratio: 1-10
**Stage 1**
Design of new reactor
1.4Mtons/year
Gaoqiao, Shanghai

**Stage 2**
Optimizing & troubleshooting
1.4Mtons/year
Yanshan, Beijing

**Stage 3**
Scale-up with aid of virtual process engineering
8Mtons/year
On blueprint, China

**SINOPEC (MIP)**
Clean gasoline production scaling-up and optimization

Novel FCC Riser
Height: 40 m
Diameter: 1~3.5 m
Determine design parameter
Diameter
Velocity
Inventory

MIP: Maximizing Iso-Paraffin
Cooperation:

Shell
GE
Unilever
Total
BASF
Alstom
BHPB
BP
Baosteel
Sinopec
PetroChina
Yankuang
Shenhua
Jincheng Coal
Synfuels China
Past

CPU Parallel

Present

CPU + GPU Parallel

Future:

xPU

Virtual reality

Breakthrough at mesoscale

Complete similarity

Problem Modeling
Software Hardware

Factory

Simulator
Virtual Process Engineering Center

1 Minute Process
1 Week Computation

3D full-loop
8s/day

4000 Cells, 45000 Particles, ms/step

1CPU + 1GPU (K20) Realtime Simulation!
What is the key to realtime simulation?

Theoretical capacity

Real capability

$X = \{ x_1, x_2, \ldots, x_n \}$

min $E_k (X)$

s.t. $F_i (X) = 0, \ i = 1, 2, \ldots, m$
Towards Mesoscience
An Transdisciplinary Science
Rationale for Mesoscience:

- **Common physical principle:** *Compromise in competition*

- **Unified Mathematical Formulation:** *Multi-objective variational*

- **Capability in applications**
  - *Predictability of physical modeling*
  - *Scalability of computation*
Summary of mesoscale complexity: 

Possible common principle

Complex world

- Phenomena
  - Heterogeneity in space and time
  - Many-body effects
  - Collective behavior
  - Self-assembly or organization
  - Uncertainty
  - Dissipative structures
  - Nonlinearity
  - Non-equilibrium
  - Emergence
  - Criticality
  - Intermittency
  - Chaos

- Feature in science
  - Complexity science
  - Multiscale modeling
  - Dissipative structure theory
  - Synergetics
  - Scaling and renormalization
  - Coarse graining
  - Constitutive, statistics, wavelet

System: Holism

Bridge: Mesoscale

Element: Reductionism

Mesoscience

Physical principle:
Compromise in competition between dominant mechanisms

Mathematical formulation:
Multi-objective variational problem

Universality


Critical: **Levels and scales**

Level-specific, distinct dominant mechanisms, but following the common principle of compromise in competition.

Major research plan on Mesoscience

NSFC 2012

Under discussion, only at mesoscopic

DOE

http://www.nsfc.gov.cn/publish/portal0/tab88/info23556.htm

http://www.sciencemag.org/content/335/6073/1167.full
Joint Virtual Special Issue

“Towards Engineering Mesoscience”

- Chemical Engineering Science
- Powder Technology
- Particuology

Towards Engineering Mesoscience

A joint Virtual Special Issue of Chemical Engineering Science, Powder Technology and Particuology

Introduction

Over many years, chemical engineers have become more aware of the complementary molecular aspects of chemical engineering, in a swing to the smaller molecular scale. The complementarity of molecular and process phenomena in the context of product design, the so-called molecule-process-product triplet elaborated eloquently by Charpentier and colleagues [CES2002a; CES2004a], has led to an enhanced understanding of molecular phenomena and the use of sophisticated tools within chemical engineering, for example molecular simulation. Yet we feel the time has come to recognize the space in between the molecular and process scales, and recognize that the interaction between length scales occurs via the mesoscales. In essence, we see the role of the meso-structure as a foundation stone complementary to molecule, for product development via process engineering.
Physical Chemistry
Multilevel and Multiscale
Mesoscales are the Path

TRANSDISCIPLINARITY: Way 1
across different sub-disciplines in the same field

TRANSDISCIPLINARITY: Way 2
across different disciplines

TRANSDISCIPLINARITY: Way 3
across global issues

GLOBAL ISSUES
Discipline
Interdiscipline

Chemical Science
Physical Science
Biological Science
Information Science
Neurological Science
Space Science
Geological Science
Social Sciences
Humanities

Sub-discipline:
Chemistry
Chemical Engineering
Process System Engineering

Level:
Material
Reactor
Factory

Scale:
BS
Meso
BS
Meso
BS
Meso
BS (Boundary scale)

Mesoscale:
Interfacial and material structures
Dynamic heterogeneity in reactor
Integrated units

Physical Chemistry
Chemical Biology
Biological Physics
Bioinformatics

Big data
Cloud/Supercomputing
Virtual Reality

Multi-scale world

Complexity

Compromise

Diversity

Common principle

Bridge

Macro-behavior

The next big thing
Discussed with:

Mathematicians
Physicists
Chemists
Biologists
Meteorologists
Astronomers
Social Scientists

Mesoscience is a common language!
Key to Mesoscience: *Transdisciplinarity*

Knowledge Integration

*VENDORS SELL PIECES.*

*PARTNERS PROVIDE SOLUTIONS.*
Thanks for your attention!