Nanoinformatics for Scale-up Nanomanufacturing: Some Studies

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October 15th, 2013
Informatics for Nanomanufacturing, Philadelphia, PA

Outline

- Study on Process Scale-up Modeling: lab-scale model vs. full-scale model for manufacturing
- Study on Understanding Process Physics under Large uncertainties
- Summary: Integrated Nanomanufacturing and Nanoinformatics

Scale-up Methodology [Xu et al., 2013]

C1. Scale-up process research: Identifying and developing NM processes and processing techniques with the potential of economical production at commercial scale, and

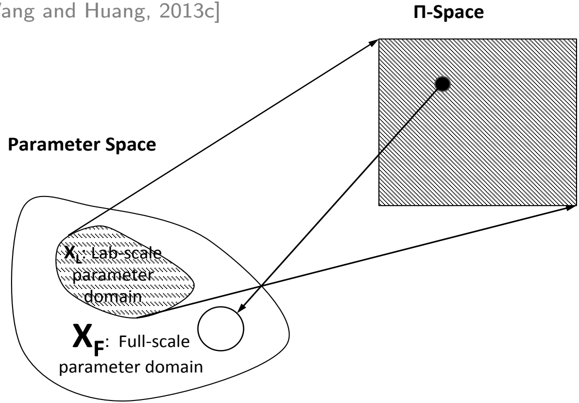
C2. **Scale-up system-level research**: Establishing modeling, simulation, and control methodologies that enable and support economical production at commercial scale: [Xu et al., 2013]

	Quantity **1 →N**	**Size** **S → L**	**Throughput** **S → F**	**Yield** **L → H**
Objective	from one to many	from small to large size or area	from slow to fast processing rate	from low to h quality
Nature of problem	improve process repeatability	scale size up	increase production rate	reduce defects
Measure of outcome	large number of units with low variations	full-scale geometry at full-scale system	short production cycle	low fraction n conforming, defect rate
Methods	variation reduction	dimensional analysis	process design	process & qua control

1. Study on Process Scale-up Modeling

- Engineering processes often are scale-dependent: lab-scale vs. full-scale.
- Predicting the full-scale process using the lab-scale model has the risk of extrapolation.
- Dilemma of scale-up process modeling:
  how to avoid model extrapolation?

Basic Idea: Transformation between Parameter Space and Π-Space [Wang and Huang, 2013c]

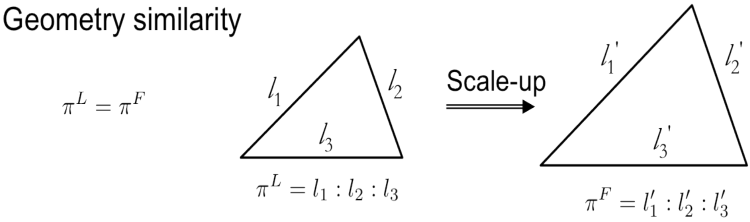


- Model interpolation maintained in the Π-space
- Extrapolation when transformed back to parameter space

How to Accomplish the Transformation

- The model in the transformed Π-space should preserve the similarity between lab-scale and full-scale models.
- The science base of achieving the scalability of engineering models is the scaling law [Barenblatt, 2003].
- The scaling law refers to the existence of a power-law relationship between variables y and x through $y \propto x^{\alpha}$.
- The law signifies the property of an engineering phenomenon: *physical similarity*, which is a generalization of the concept of *geometric similarity*.

Geometric Similarity and Transformation



- The ration $\pi = l_1 : l_2 : l_3$ is a transformation from parameter space $\{l_1, l_2, l_3\}$ to *Pi*-space $\{\pi\}$.
- Similarity will be preserved if the ratios are the same

Physical Similarity and Transformation

The **parameter space** of an engineering process:

physical quantities $(y, x_1, x_2, \ldots, x_p)$:

- Geometric parameters: e.g., diameter of MOCVD chamber
- Physical properties: e.g., density, viscosity
- Process parameters: e.g., flow rate, temperature

The Π-**space** of an engineering process:

- π_i's: proper combinations of physical quantities $\Longleftrightarrow$ length ratio $\pi = l_1 : l_2 : l_3$
- Two physical processes are *complete similar* if $\pi_i^L = \pi_i^F \Longleftrightarrow l_1 : l_2 : l_3 = l_1' : l_2' : l_3'$.

Dimensionless π numbers and Dimensional Analysis (DA)

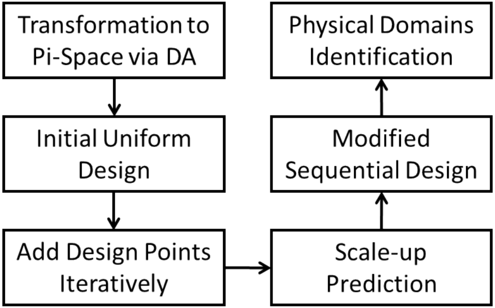
- π_i's are derived through dimensional analysis (DA) [Buckingham, 1914, Bridgman, 1922, Sedov, 1993, Taylor, 1974, Szirtes, 2007].
- Essential idea: physical laws have the property of dimensional homogeneity, i.e., additive terms in the functions will have the same dimensions or units.
- This property allows the number of arguments in the mathematical expressions to be reduced, thus making them simpler to obtain either from theories or experiments
- Popular methods: Rayleigh's method, Buckingham Π-theorem , matrix method, and method of synthesis [Rayleigh, 1915, Buckingham, 1914, Sharp, 1981, Zlokarnik, 1991].

Related Work: DOA and Dimensional Analysis (DA)

- Combining DA and statistical modeling of LP-CVD [Wehrle, 1989]
  - Derived dimensionless groups governing LP-CVD
  - Fitted polynomial regression models both for $\pi = \Phi(\cdot)$ and the primitive process variables.
- Combining the DA and statistical DOE for a hydrodynamics experiment on the thrust of a propeller [Islam and Lye, 2009]
  - DA reduced 14 variables to 11 dimensionless numbers π_i's
  - A two-level fractional factorial design was used to screen out insignificant π_i's
  - Response surface modeling established a functional relationship between the dependent dimensionless thrust coefficient and the remaining five significant π_i's.
- Statistician's effort to combine DA and statistical DOE [Albrecht et al., 2013]
  - Assumed a third-order regression model for $\pi = \Phi(\cdot)$
  - D-optimal design proposed to experimentally investigate $\pi = \Phi(\cdot)$
  - Robustness regarding missing physical quantities and optimization considered

Engineering Design of Scale-up Experiments and Model Building: Objective & Proposed Procedure [Wang and Huang, 2013c]

- Objective: Identifying the scaling law and its physical domain
- Proposed Procedure:



Scale-up Engineering Experimental Design Example

Response F_D: the drag force on a smooth sphere in a uniform fluid

Factors:

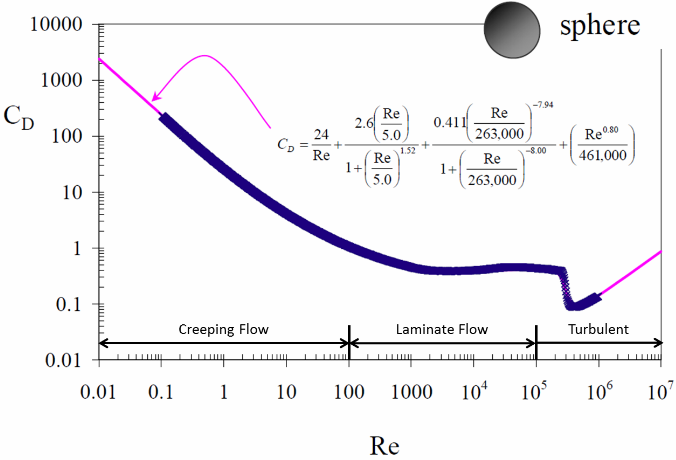
- R: Radius of the sphere
- v: Velocity of the sphere
- ρ: Density of the fluid
- μ: Dynamic viscosity of the fluid

True physical model from fluid dynamics [Schlichting and Gersten, 2000]

$$F_D = \frac{1}{2} C_D \; \rho \; v^2 \; (\pi R^2)$$

Drag coefficient C_D: depending on Reynolds number $Re = Rv\frac{\rho}{\mu}$

Drag Coefficient C_D vs. Re



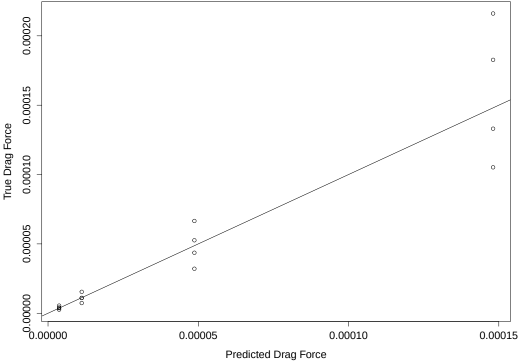
Not Knowing True Physical Model for Scale-up Experiment

Traditional Full Factorial Design: a full factorial 2^4 design

Table: *Factor Levels for Factorial Design*

Factor(Unit)	**Low**	**High**
Radius(Meter)	0.01	0.05
Velocity(Meter/Second)	0.005	0.01
Density(Kilogram/Cubic Meter)	500	1000
Viscosity(Pascal · Second)	0.0004	0.00089

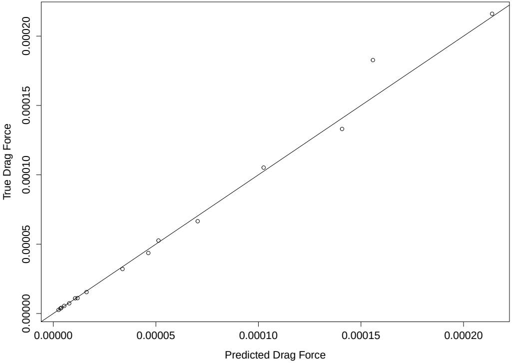
Full Factorial 2^4 Design: Log Transformation of Response



- R^2=0.964, problematic prediction with large drag force
- Missing critical factors of density ρ and viscosity μ
- not scalable

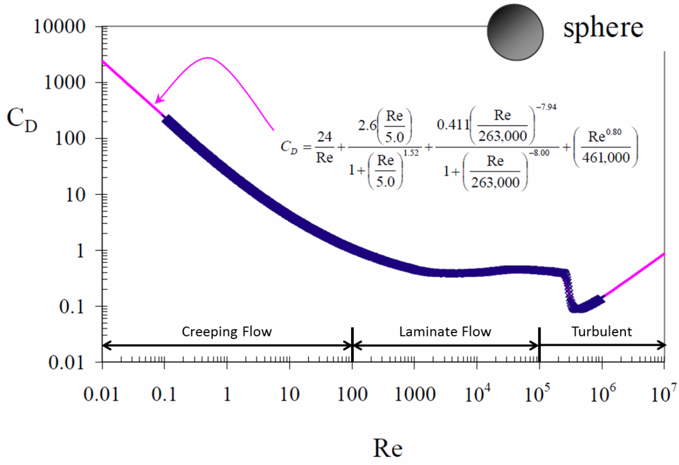
Modeling Building in the *Pi* Space

$$\log(\frac{F_D}{\rho(Rv)^2}) = \beta_0 + \beta_1 \log(\frac{Rv\rho}{\mu}) + \varepsilon \qquad (1)$$



True drag force versus predicted values with $y = x$ straight line after DA

Sequential Engineering Design of Scale-up Experiments for Exploring Multiple Physical Domains



Sequential Engineering Design of Scale-up Experiments

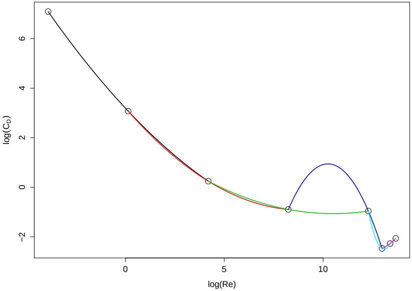
- Idea: concentrate more on the region where the relationship between Re and C_D changes.
- Approach: Fit a series of simple functions g_i in moving windows of k observations, then we compare the consecutive g_i and g_{i+1} and put the new design point where g_{i+1} is most different from g_i.
- Measure: Use the L2-distance $D = \sqrt{\int (f-g)^2 \,\mathrm{d}x}$ as a measure of dissimilarity between g_i.

Fore the series of g_i, we choose second order polynomial function as it requires only three data points in each window but still able to approximate non-linear behaviors.

Modified Sequential Design for Drag Experiment

Table: *Second Quadratic Fittings and L2-Distance between* g_i^j [Wang and Huang, 2013c]

Window i	a_i^2	b_i^2	c_i^2	D_i
1	3.19	-0.855	0.0362	NA
2	3.20	-0.920	0.0513	0.163
3	2.55	-0.689	0.0328	52.1
4	-61.1	12.2	-0.596	1.37E4
5	237	-35.6	1.32	2.69E4
6	501	-76.9	2.93	3.52E4
7	52.2	-8.77	0.351	**4.91E4**



Study on Scale-up Process Modeling: Summary

- Transformation through dimensional analysis is the key for scale-up experiment and modeling building.
- The sequential design supports the scale-up experiment well with limited experimental efforts.
- The design will be harder for high-dimensional Π space
- Dimensional analysis for complex processes such as nano fabrication processes is challenging.

2. Study on Understanding Process Physics under Large uncertainties [Huang, 2011b, Huang et al., 2011, Wang and Huang, 2013b, Xu and Huang, 2012, Xu and Huang, 2013]

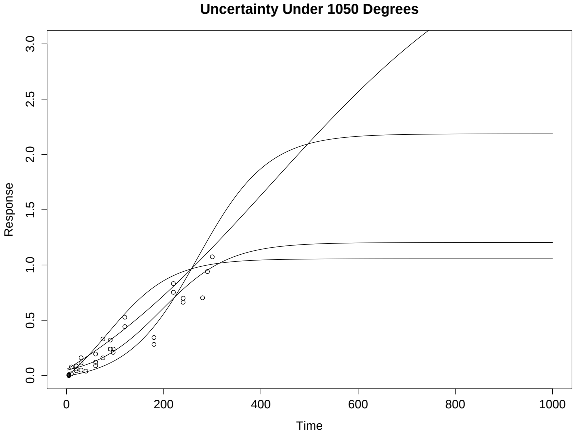
Large uncertainties involve in modeling nanomanufacturing processes:

- Uncertainties in physical understanding of process physics.
- Uncertainties in data collection: limited data, large variations among experimental runs
- Dilemma of scale-up process modeling:
  how to obtain credible understanding of process physics?

Large Uncertainties: An Example in Nanowire Growth

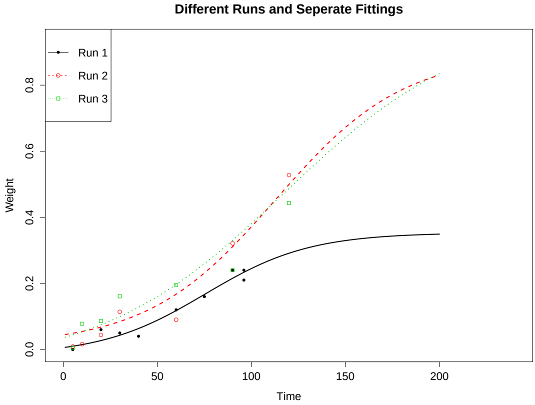
A large pool of statistical models fit the data equally well

[Wang and Huang, 2013b]

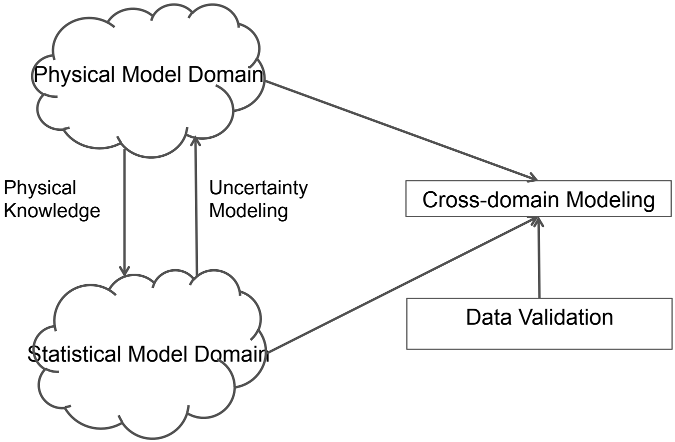


Large Uncertainties: An Example in Nanowire Growth

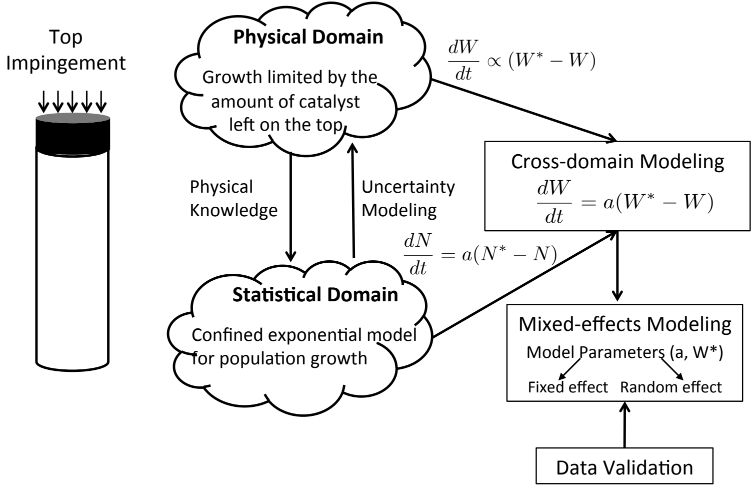
Models for different runs can be different as well due to large variations among nano experimental runs [Wang and Huang, 2013a]:



Cross-Domain Model Building and Validation (CDMV)

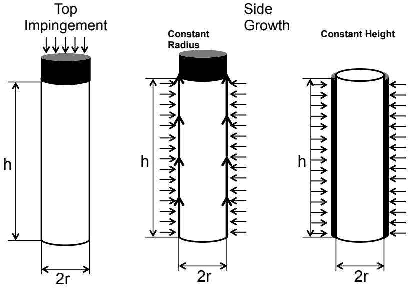


Cross-Domain Model Building and Validation (CDMV)



Cross-Domain Model Building and Validation (CDMV)

$$\frac{\mathrm{d}W}{\mathrm{d}t} = \gamma_1(W^* - W) + \gamma_2 W^{\alpha}(W^* - W) \tag{2}$$



- Identified the contributions of two growth mechanisms under each growth condition (γ_1 vs. γ_2) [Wang and Huang, 2013b].
- Identified the changes of contributions under two growth conditions

Summary

Scale-up Nanomanufacturing relies on informatics, more important on the integration of nanoinformatics and nanomanufacturing [Huang, 2011a]

Acknowledgement

The work is supported by National Science Foundation with CAREER NSF CMM-1055394, CMMI-1000972, and CMMI-0728100

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