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Process Modeling: where to next? 2040 visions of Process Systems Engineering

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- Process Modeling: where are we now?
- Process Modeling: where to next ?
- Concluding remarks



Where are we now?

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Dimensions of process modeling





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Process Modeling Key drivers

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Use validated models that are predictive over wide ranges of design & operating parameters increase reliability/reduce risk in model-based decisions



Leverage modeling investment across process lifecycle → ensure consistency, reduce cost of model development & maintenance

Integrated gas production & processing networks Basrah Gas Company





D. Aluma, N. Thijssen, K.M. Nauta, C.C Pantelides, N. Shah "Optimize an integrated natural gas production and distribution network" *Gas Processing News*, October 2016.



Integrated gas production & processing network Top-level model



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Integrated gas production & processing network

Second-level models







Where to next ?

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Process modeling: where to next? Increasing the efficiency of the modeling process

Model-based Engineering



Business Objectives

Model-based Engineering

Business Deliverables

Model-based Engineering





Analysis of business objectives Formulation of modeling approach Model construction Correctness testing

Model validation

Model-based calculations for process analysis & optimization

Application deployment

Business Deliverables

Model validation





Model validation Characterization of fundamental physical phenomena

- Most process models contain parameters that are not known a priori
 - thermodynamics
 - heat & mass transfer
 - hydrodynamics
 - reaction & other kinetics

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- Typically estimated from experimental data
- Experimentation almost always the bottleneck in terms of time & cost
 - design experiments carefully
 - extract maximum amount of information from this exercise



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ALTERNATIVE: multiscale modeling





Cocrystal lattice energy

CrystalOptimizer

landscape in CrystalPredictor/

Ibuprofen model in SAFT-γMie



CFD model of agitated solid/liquid reactor for drug substance manufacturing

Multiscale modeling: an *old* "new paradigm"! So what are the challenges for 2040 ?



1. Scope of fine-scale models

 Do they cover the physical phenomena of interest to process modeling?

2. Accuracy of fine-scale models

 Is the accuracy of characterization of these physical phenomena comparable to what can be obtained by estimation from experimental data?

3. Efficiency of multiscale integration

 Can problems of practical significance be solved? What, if anything, canProcess Systems Engineering contribute to these?

Process Systems Engineering methodologies



Multiscale modeling: a not (yet) successful example <u>Prediction</u> of solubility for process modeling

Fine-scale modeling: Ab initio crystal structure prediction



BUT... currently ab initio available methods

- not (yet) applicable to molecules of practical significance
- not (yet) accurate enough

Process modeling: where to next? Beyond manufacturing



Dimensions of process modeling





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Pharmaceutical systems



Decisions & Disturbances

Critical Process Parameters (CPPs)



Objectives & Constraints

Product KPIs: Critical Quality Attributes (CQAs)

© 2017 Process Systems Enter Process KPIs: Economics, Safety, Operability, Environmental Impact

Pharmaceutical systems



Decisions & Disturbances

Critical Process Parameters (CPPs)



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Product KPIs: Critical Quality Attributes (CQAs)

© 2017 Process Systems Enter Process KPIs: Economics, Safety, Operability, Environmental Impact

Systems-based Pharmaceutics

The vision





Use an <u>integrated system model</u> to quantify effects of CPPs & disturbances on CQAs, process economics, operability, safety
– incorporate all available knowledge, identify gaps
Maximize efficiency of new drug development

Systems-based Pharmaceutics

Process Systems Engineering tools & workflows





Process modeling: where to next?

From point calculations to global process understanding

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Model-based process system analysis

Current practice





Model-based process system analysis Global system behavior in an uncertain world





Model-based process system analysis Global system behavior in an uncertain world







Global sensitivity indices of output response(s) with respect to input factors

Global System Analysis Some interesting questions





Relation with optimization-based methodologies?



Process modeling: where to next? In conclusion...



Process modeling: What next?



Potential major developments

- Multiscale modeling
 - accelerating model development via reduced reliance on experimentation
- Combined process & product performance modeling
 - taking direct account of end-use product performance in manufacturing process design & operation

Global system analysis

 extracting maximum insight from modeling investment

Impact of enabling infrastructure

High-Performance Computing

- ensuring scalability of existing types of calculation
- enabling new types of calculation
- Cloud Computing
 - High-Performance Computing
 - see above
 - Data accessibility
 - much reduced effort for collection of data underpinning models
 - elimination of most manual data entry
 - a <u>data-centered</u> world: model-based calculations effect data transformations

Profound implications on architecture & design of process modeling software





Questions?

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Model-based automation





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Process modeling technology Original vision: multipurpose process modeling environments





Process modeling technology A new paradigm

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