Be Careful What You Wish For:

Some thoughts on maximizing value from your simulations

Scott J Bury, PhD

Engineering & Process Sciences R&D

The Dow Chemical Company

Presented at the 2014 CMU EWO Seminar

Jan 23, 2014

WORLDWIDE PARTNER

Agenda

- Dow at a Glance
- Slices of Simulation at Dow
- Discrete Event Simulation
- What Engineers should about what it takes to deliver value from a simulation
- The Importance of Cows in Simulations

Who We Are

Combine the power of science and technology to passionately innovate what is essential to human progress

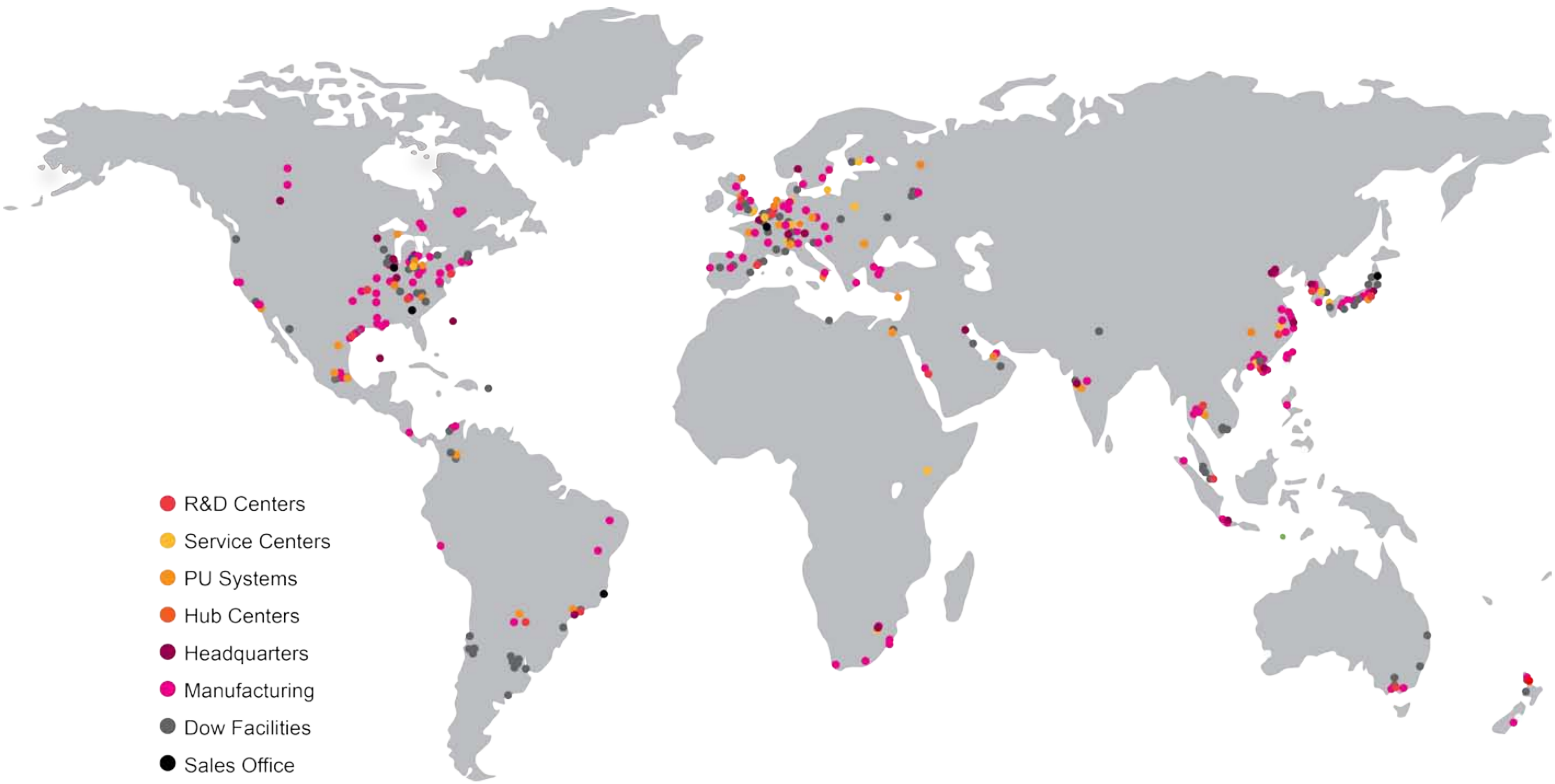
1897 Founded by Herbert H. Dow in Midland, Michigan

~160 Countries in which we serve customers

More than **5,000** products are manufactured at **188** sites in **36** countries

54,000 Approximate Employees worldwide

Dow Locations



Vision, Strength and Focus

Vision

To be the most profitable and respected science-driven chemical company in the world

Mission

To passionately innovate what is essential to human progress by providing sustainable solutions to our customers

Values

- Integrity
- Respect for People
- Protecting Our Planet

Innovation in Action

Through meaningful, science-based innovation and strong collaboration, Dow is delivering the value our customers want and the world needs.

- Helping achieve higher yield potential through plant biotechnology
- Enabling better quality in electronic displays and general lighting
- Tackling water challenges in a sustainable way

2012 Innovative Milestones

412 U.S. patents granted to Dow in 2012

Dow R&D features an elite team of nearly **7,000** employees globally

$7 billion Net Present Value of R&D projects in commercialization

Dow's Diverse and Integrated Portfolio

ELECTRONIC & FUNCTIONAL MATERIALS

- Dow Electronic Materials
  - Semiconductor Tech
  - Interconnect Tech
  - Display Technologies
  - Growth Technologies
- Functional Materials
  - Dow Wolff Cellulosics
  - Dow Consumer & Industrial Solutions
  - Dow Microbial Control
- JV: Dow Corning Corporation

COATINGS AND INFRASTRUCTURE SOLUTIONS

- Dow Building & Construction
- Dow Coating Materials
- Dow Water & Process Solutions
- Performance Monomers
- JV: Dow Corning Corporation

AGRICULTURAL SCIENCES

- Dow AgroSciences
  - Agricultural Chemicals
  - Seeds, Traits & Oils
  - Crop Protection

PERFORMANCE MATERIALS

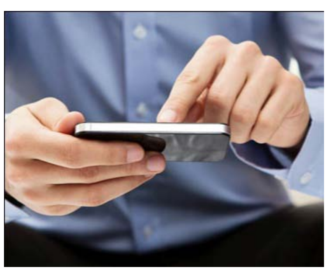
- Amines
- Chlorinated Organics
- Dow Automotive Systems
- Dow Formulated Systems
- Dow Oil & Gas
- Dow Plastics Additives
- Epoxy
- Oxygenated Solvents
- Polyglycols, Surfactants & Fluids
- Polyurethanes
- Propylene Oxide/Propylene Glycol
- JV: Map Ta Phut
- JV: MEGLOBAL
- JV: Sadara Chemical Company

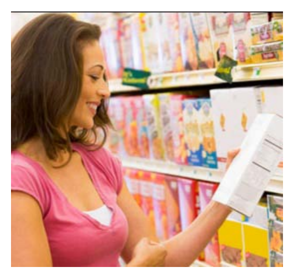
PERFORMANCE PLASTICS

- Dow Elastomers
- Dow Electrical & Telecommunications
- Dow Hygiene & Medical
- Dow Performance Packaging
- JV: EQUATE Petrochemical Company K.S.C
- JV: The Kuwait Olefins Company K.S.C.
- JV: The SCG-Dow Group
- JV: Sadara Chemical Company

FEEDSTOCKS AND ENERGY

- Chlor-Alkali/Chlor-Vinyl
- Energy
- Ethylene Oxide/Ethylene Glycol
- Hydrocarbons
- JV: EQUATE Petrochemical Company K.S.C
- JV: The SCG-Dow Group
- JV: The Kuwait Olefins Company K.S.C

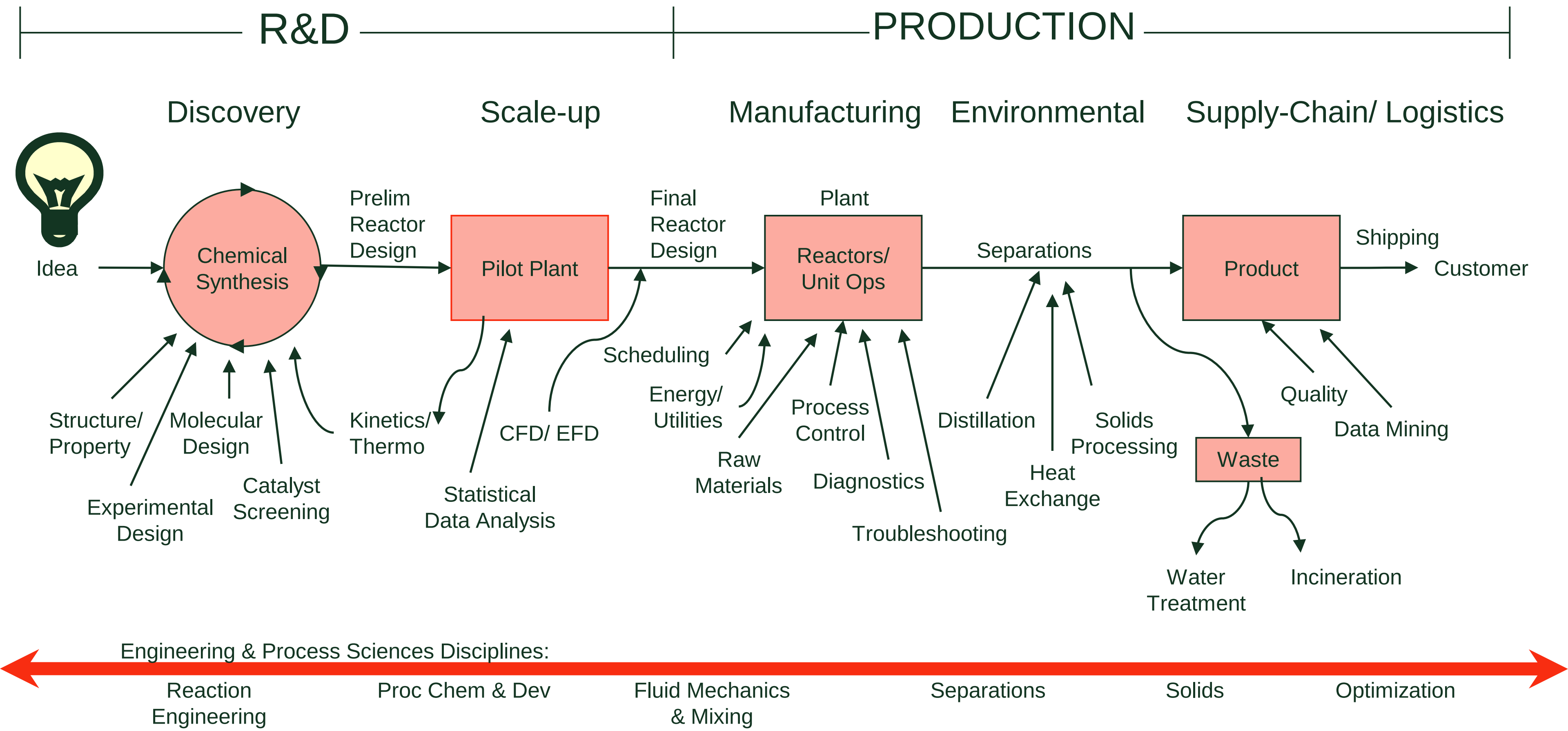


Agenda

- Dow at a Glance
- Slices of Simulation at Dow
- Discrete Event Simulation
- What Engineers should about what it takes to deliver value from a simulation
- The Importance of Cows

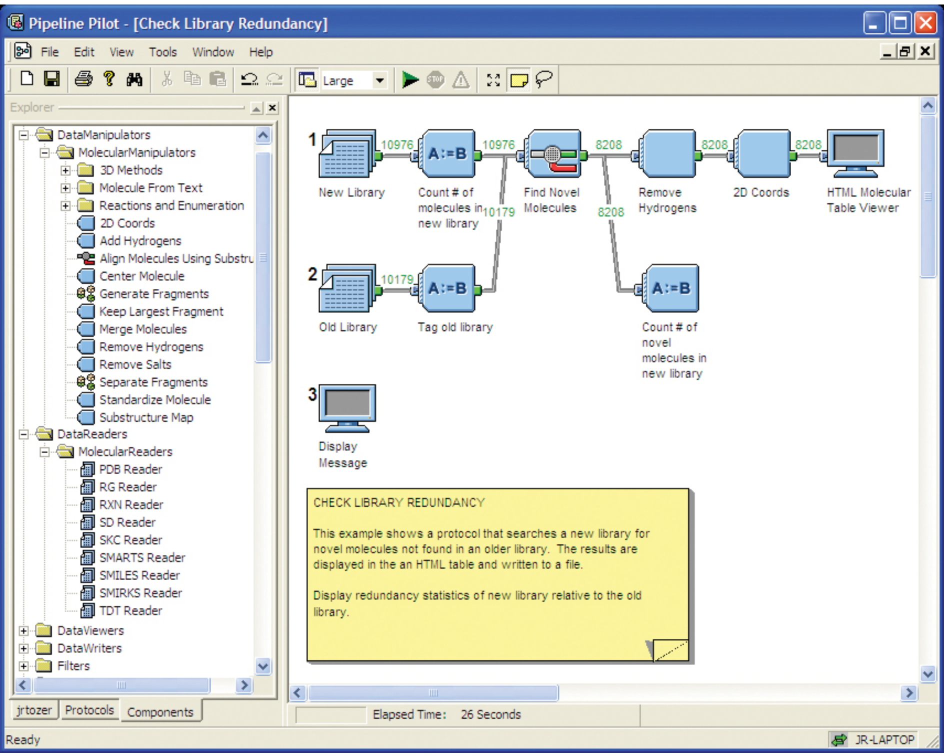
Simulation Touch Points in Chemical Production

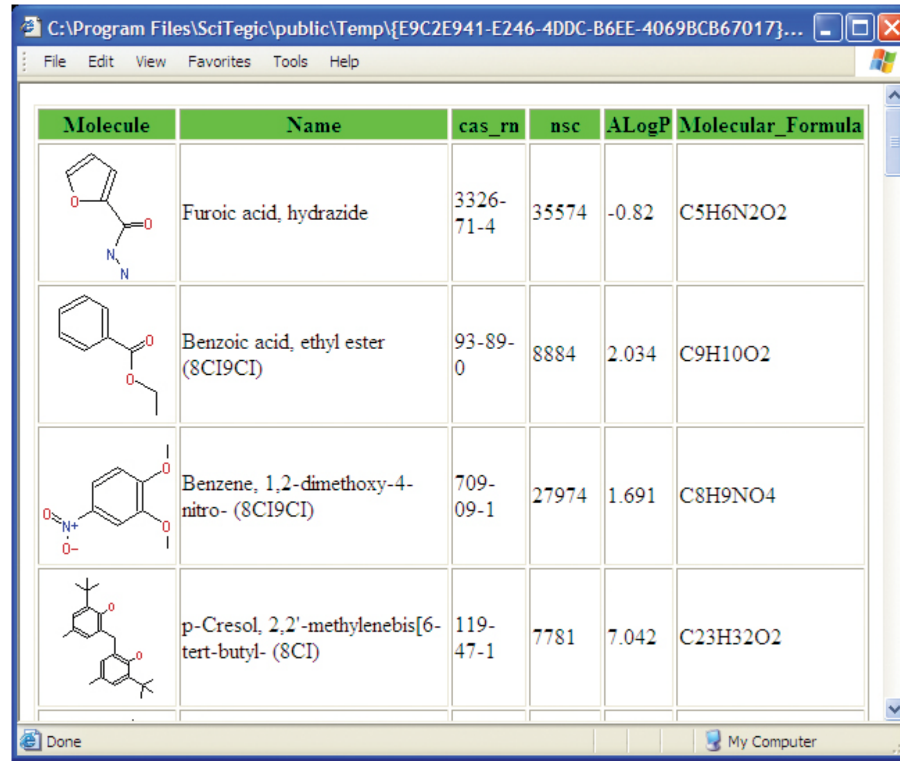


Adapted from *Modeling Challenges in Process Development (Chemical Industry Perspective)*, Alex Kalos, Presented at a two-day workshop organized by the Pharmaceutical Industry and the Council for Chemical Research, University of Maryland Biotechnology Institute (UMBI-Shady Grove, Rockville, MD), June 7-8 (2007). See CRI DOC 19723.

DOW®

Simulation at the Molecular Level

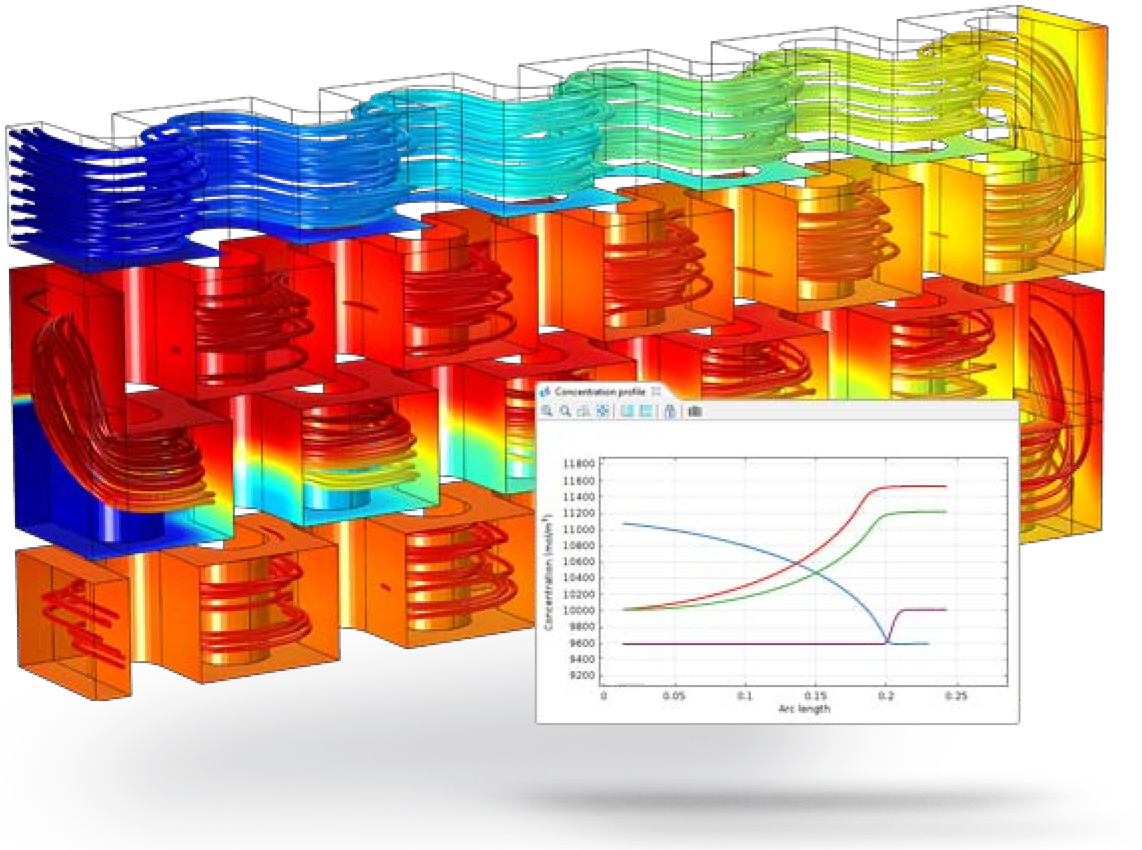




Molecule	Name	cas_rn	nsc	ALogP	Molecular_Formula
	Furoic acid, hydrazide	3326-71-4	35574	-0.82	C5H6N2O2
	Benzoic acid, ethyl ester (8CI9CI)	93-89-0	8884	2.034	C9H10O2
	Benzene, 1,2-dimethoxy-4-nitro- (8CI9CI)	709-09-1	27974	1.691	C8H9NO4
	p-Cresol, 2,2'-methylenebis[6-tert-butyl- (8CI)	119-47-1	7781	7.042	C23H32O2

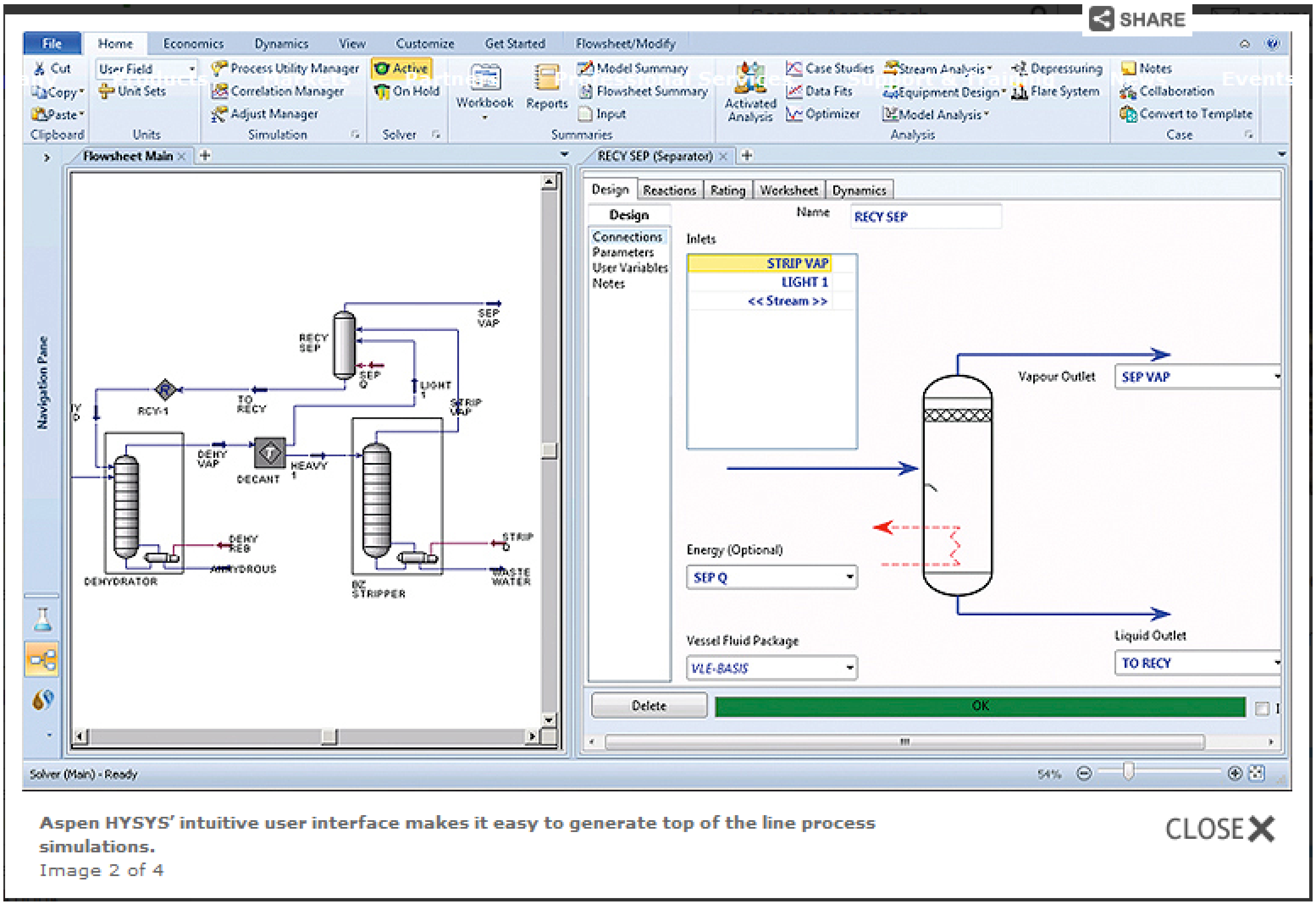
Source: http://accelrys.com/products/pipeline-pilot/component-collections/chemistry.html
Accessed Oct 2013

Simulation at the Unit Ops Level (Physics and Chemistry)



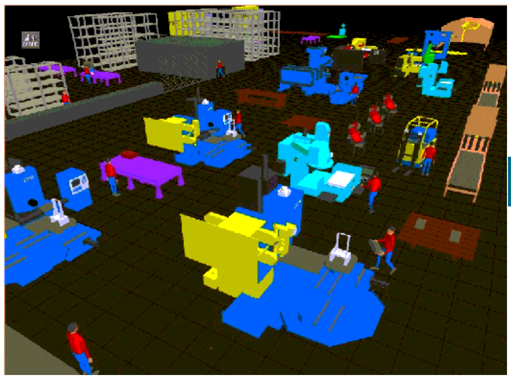
Source: http://www.comsol.com/chemical-reaction-module

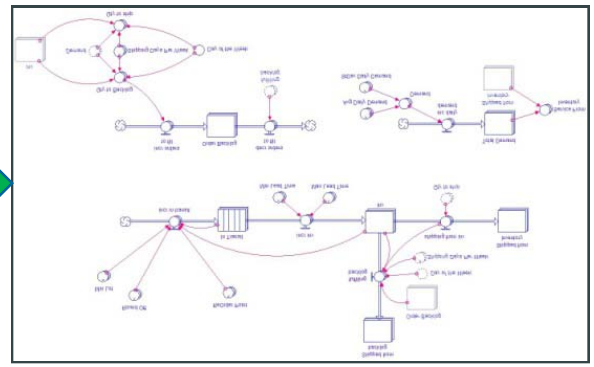
Traditional Process Flowsheets

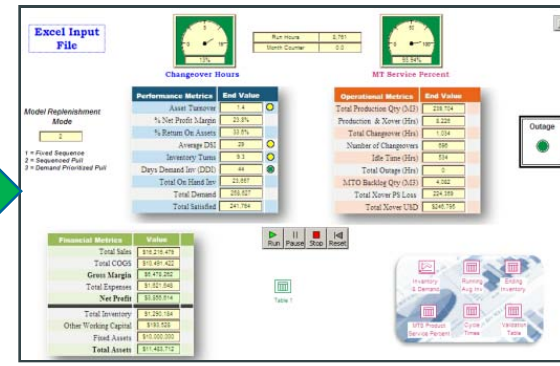


http://www.aspentech.com/products/aspenone-engineering/

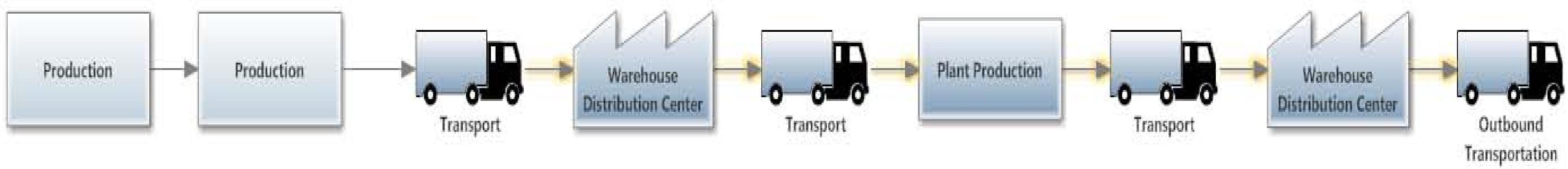
Simulation at the Plant Floor







Simulation at the Enterprise Level



Reliability Engineering

Manufacturing & Operations

Business Strategies

Supply Chain

Economic Data

Decision Support Models

The modeling approach integrates upstream (production, reliability) and downstream (demand, variable margins) information for decision-making purposes

Agenda

- Dow at a Glance
- Slices of Simulation at Dow
- Discrete Event Simulation
- What Engineers should know about what it takes to deliver value from a simulation
- The Importance of Cows in Simulations

The modeling traditions for each of these inputs are different

Reliability & Maintenance – Component and Asset focused.

Asks does the system fail before end of Mission Time
Uses Weibull Analysis, can have1000's of components and extreme detail and long mission times, Stochastic

Operations and Manufacturing – Industrial Engineering Influenced discrete event

Asks what is the throughput and where are the bottlenecks?
Traditionally uses discrete items, random numbers, queues & activities, Stochastic and typically time scheduled. Can be either finite or steady-state

Business Strategies – System Dynamics (The Forrester tradition)

Asks how does the system change over time.
Models the word as stocks and flows with feedback loops (ODE's).
Usually deterministic and run open loop. Can become a bit odd when they try to be discrete event

Supply Chain – Mix of SD and DES

Economic Data – Statistical and Time Series Models

The software platform will influence the simulation development and work process

“People can be extremely loyal (fanatical?) about their tool of choice*”

I have seen people nearly come to blows over “the right way to handle discrete event statistics” – sort of like the RTN vs STN formulation question

I have been told that a software platform cannot be used for reliability modeling because it doesn’t automatically calculate a particular metric like the their current tool

For stochastic simulations conflicts can arise from different philosophies on random number generation, use of seed streams, whether seed streams as variance reduction is even valid and necessary.

*including your speaker

Some DES approaches we have found useful for Chemical Plants

How to mix efficiently combine continuous flow and discrete events?

Discrete Rate Technology (for example ExtendSim) is very effective. It models flow or high rate items (100’s of widgets/min) as network flow LP’s. These segments can be solved very efficiently and allow for sophisticated stream handling.

Allows for layering of scheduling and control logic as well as the reliability and maintenance events on top as discrete event models.

Allows for ready conversion from flow to discrete items like ships, barges, and railcars or from batch units to flow units or raw material supplies to batch units.

Especially useful for larger networks

Gaining flexibility in the simulations?

Database driven models provide options

- Generic Structures

- Scenario and Operating Structures

Going from Concepts to Computer Model

"Begin by modeling the data" – *Dave Krahl, Imagine That Inc., 11/3/2009*

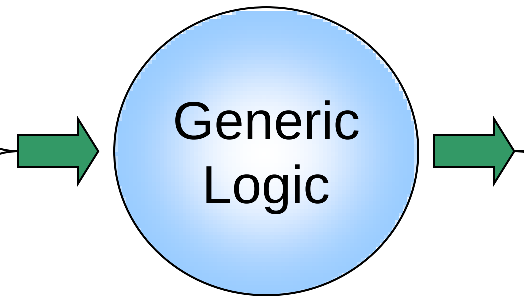
Generic simulation framework to accelerate project execution:

- Generic simulation logic that applies to a class of problems
    - Single model for **multiple systems** vs. **multiple scenarios** (of a single system)
    - Typically more Design Exploration & Testing
- Problem-specific customization by input data
- Enabled by simulation platform with database features and database aware blocks (e.g. ExtendSim™)
- Database design → model design

Example: Generic Plant Model

Input Data

Process connectivity
Production trigger
Batch sizes
Batch times and/or rates
Process/product recipes
– Resource consumption / generation
Inventory, Equipment
Operator activities
Process failures



Output Data

Throughput
Utilization statistics
- Processes
- Resources

Blocking/starving statistics
Failure statistics

- Real Dow examples of using a single model to model multiple systems:
  - Evaluation of different process configurations / technologies at the plant design and capital scoping stage
  - Evaluation of process improvements and policy changes for all plants (same process technology) in a single business

Scenario and Operating Structures for "Fixed" Assets

Flexible simulation framework to accelerate project execution:

- Multiple simulation logic that applies to a specified system
  - Single model for **multiple scenarios** vs. **multiple systems**
  - Typically more Operational focused
  - Operating in different modes with different objectives
    - For example different market demands or raw material shortages
- Problem-specific customization by input data
- Enabled by simulation platform with database features and database aware blocks (e.g. ExtendSim™)
- Database design → model design

Challenges with Simulation

What simulation gives you

How does the system performance change when I make this particular change to the system?

Combinatorial Explosion

Lots & lots of scenarios

What you really want to know

What changes do I need to make to satisfy the performance target?

Simulation Plus …

Analytical models → Explore the solution space at high level, develop scenarios to simulate

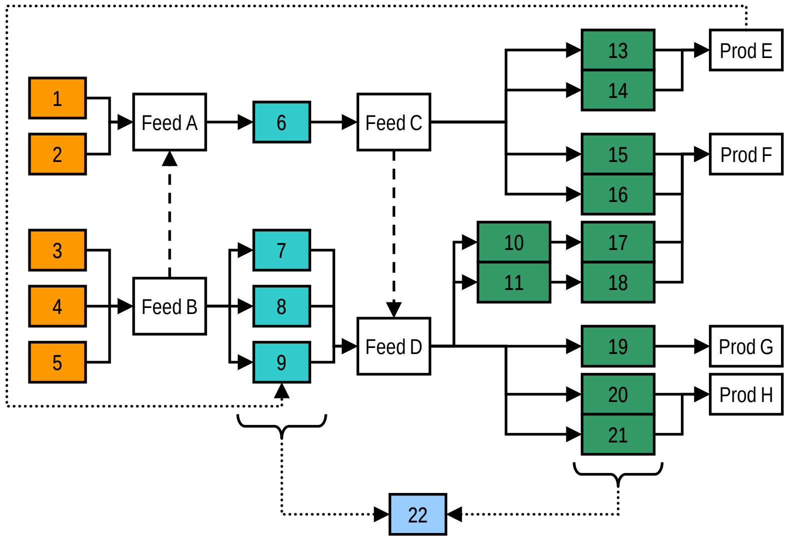
Optimization → Optimize decision variables using a simpler model, validate with simulation

Designed experiments + Response surface modeling

Indentify the interesting range of decision variables, develop scenarios to simulate

Smarter simulation
Faster decision making

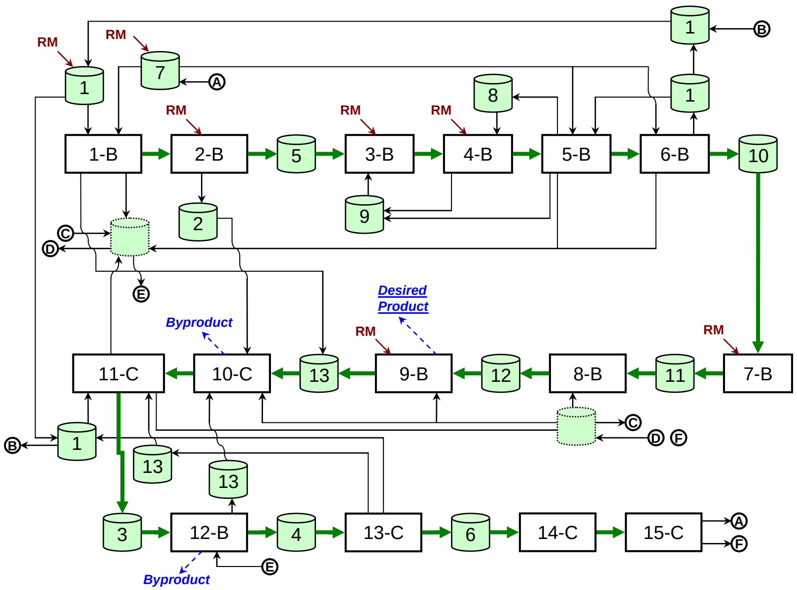
Example: Simulation + Analytical Model



This integrated plant is sold out and needs to increase throughput. All units experience frequent shutdowns. Which units need to improve and by how much? What is the priority of improvement projects?

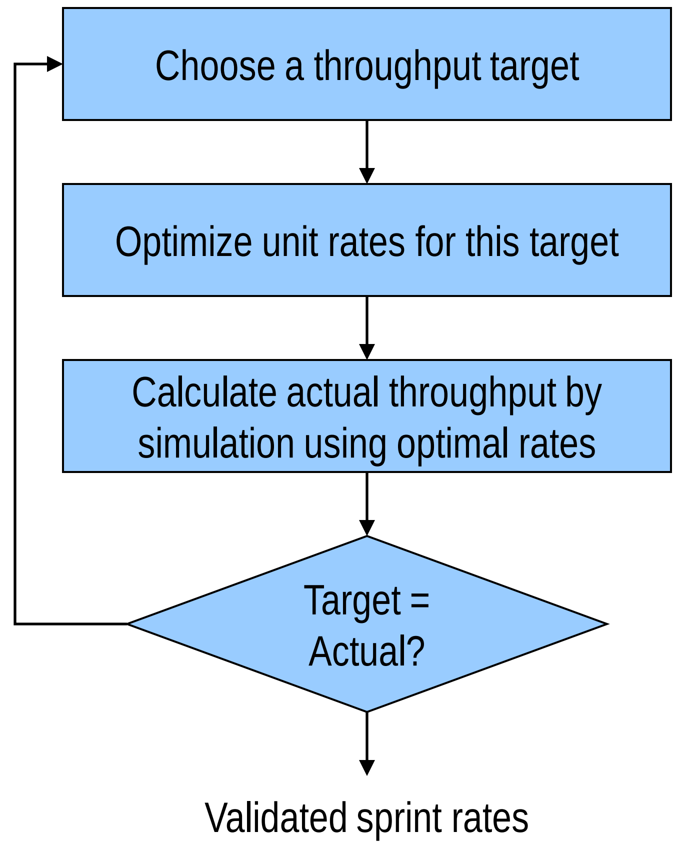
Throughput = *f*(Availability) → Opportunities identified and prioritized → Targeted simulation

Example: Simulation + Optimization

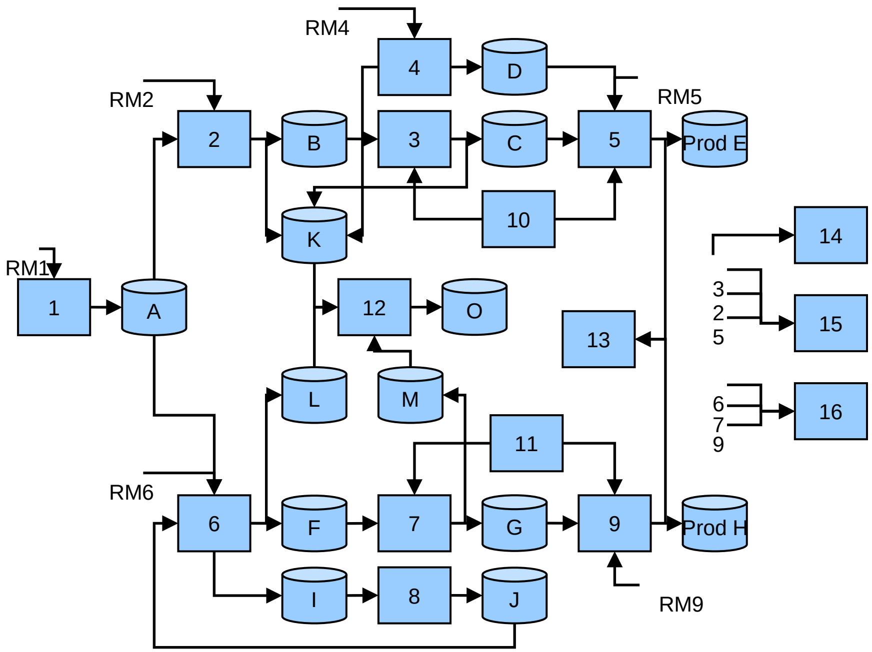


This *highly* integrated plant is sold out and needs to increase throughput. All units experience shutdowns. How much capacity increase at *each unit* should be made to attain target throughput?

Optimal rates ≡ minimum rates that are balanced and satisfy target throughput



Example: Simulation + DOE



This integrated plant is under design. What are the values of design variables (unit rates, storage capacities) that satisfy target throughput at minimum cost?

Experimental response comes from simulation.

DOE #1
Failure Parameters → High-impact units → DOE #2
Design Variables → Optimal design

Formulation of the problem easy as ABCD

- What can you **A**djust?
  - Defining what knobs we can turn
- What do we mean by **B**est?
  - Defining the correct objective function
- What **C**onstraints must be obeyed?
  - Defining the constraints (operational, legal etc)
- What is the uncertainty **D**istribution?
  - What is the right stochastic character to include?

Some technical details that I think we can do better at

- Autocorrelation or structure in input models is almost always neglected in Discrete Event simulations (I don’t know of any simulator outside some spreadsheet Monte Carol tools – that do autocorrelated inputs)
  - Appreciation of the impact on the output is important
  - Techniques needed to either de-correlate or eliminate the structure in data
  - Techniques needed to efficiently generate and use autocorrelated random numbers in the simulations
- As we model large and complex systems the number of output metrics also increases but we tend to still use a single metric to measure convergence
  - Are we making statistical invalid decisions for multiple metrics?
  - What are the implications of trying to model the failures of 1000’s of components at an hourly granularity over 20 years? Is this really needed for effective decisions? Can we develop guidelines for managing multiple metrics in complex simulations.

Agenda

- Dow at a Glance
- Slices of Simulation at Dow
- Discrete Event Simulation
- What Engineers should know about what it takes to deliver value from a simulation
- The Importance of Cows in Simulations

There are two keys to maximizing value from your simulation

Definition & Execution

See: O. M. Ülgen, S. J. Bury, R. Lu, E. J. Williams, and D. C. Wood, "Panel discussion: Business processes for applying de simulation effectively in manufacturing companies," in *Winter Simulation Conference, 2010, p. 1767.*

Some typical definitions for simulation

simulation [ˌsɪmjʊˈleɪʃən]*n*

1. the act or an instance of simulating

2. the assumption of a false appearance or form

3. (Electronics & Computer Science / Computer Science) a representation of a problem, situation, etc., in mathematical terms, esp using a computer

4. (Mathematics) *Maths statistics computing* the construction of a mathematical model for some process, situation, etc., in order to estimate its characteristics or solve problems about it probabilistically in terms of the model

5. (Psychiatry) *Psychiatry* the conscious process of feigning illness in order to gain some particular end; malingering

Collins English Dictionary – Complete and Unabridged © HarperCollins Publishers 1991, 1994, 1998, 2000, 2003

These miss the point…

DOW®

What we want is this…

Simulation (n)

A method for defining a decision about acting on something of interest and subsequently generating the required data to make the decision.

Why we should like this definition

1. Focus on the Decision and Action
   - Value follows from decisions and actions
   - Separates the important simulation projects from the nice to do
   - Applicable to any project but especially important when dealing with a “systems” project
2. Focus on the Data
   - Clarity about the decision and action brings efficiency to generating the data
3. Frees you to be a problem solver who uses models vs. “just one of those modeler types”

Your effort up-front in the definition phase pays (non-linearly) dividends in the execution phase

In Ülgen et al. I refer to Simulation Quality Objectives (SQO) modeled after the EPA's DQO process

1. State the Problem.
2. Identify the Decision.
3. Identify the Inputs to the Decision.
4. Define the Scope and Boundaries of the Study.
5. Develop a Decision Rule.
6. Understand how much Uncertainty can be tolerated in the Data.
7. Optimize the Simulation Design.

Expect that this process will take 10X the effort that you originally estimate

DOW®

Understanding the data required to make the decision

This is different than understanding the data available to build the models and simulations.

This is successful when you get the “decision maker” to commit to a decision rule

You now have clarity about the customer requirements for your product

Now you can go about delivering the product

Ensuring Business Alignment

Before jumping into the simulation tool…

- Understand the current state
- Understand the desired state

Start with the Voice of Customer:

- What decisions need to be made?
- What information is needed to make those decisions?
- What data will provide that information?
- How do we generate those data?

Gain Commitment

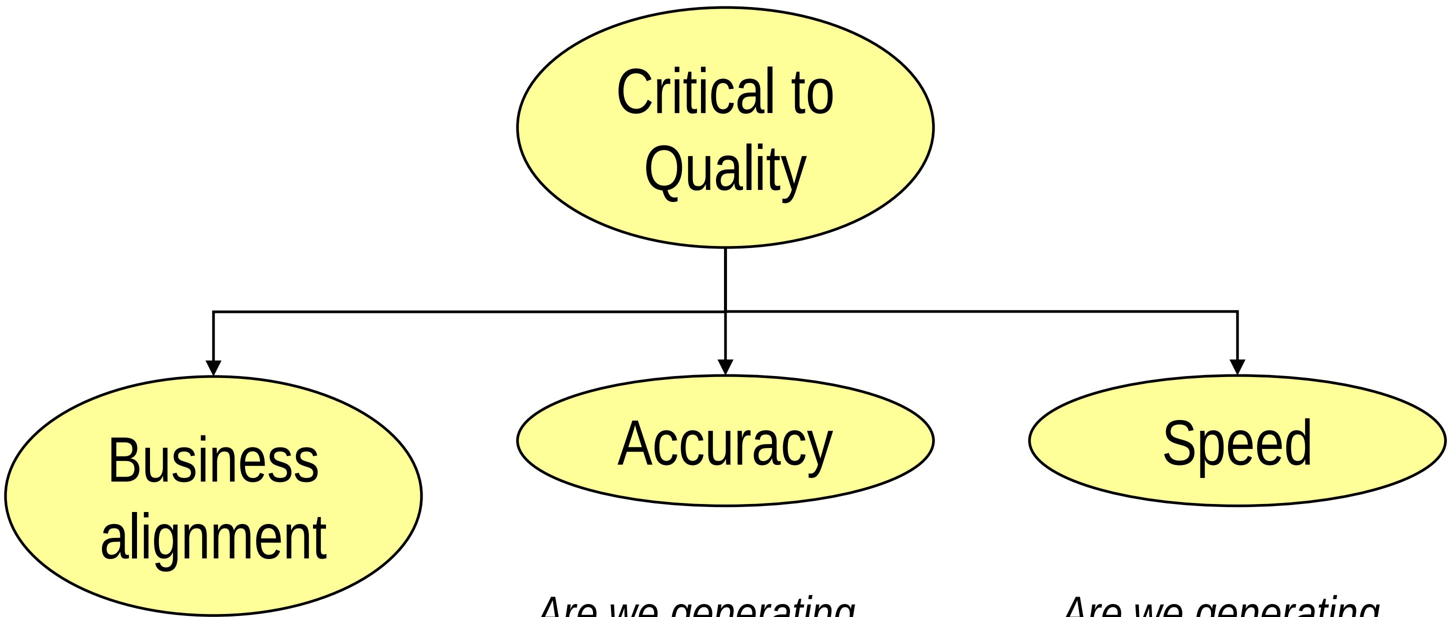
- Simulation adds complexity and effort to a project. The modeler is typically not the owner of the input data nor process knowledge. Must be supported by resources from the project team!

Doing this part well or not can make or break the project.

This happens when you skimp on the Definition phase

Execution

Decision Support with Simulation



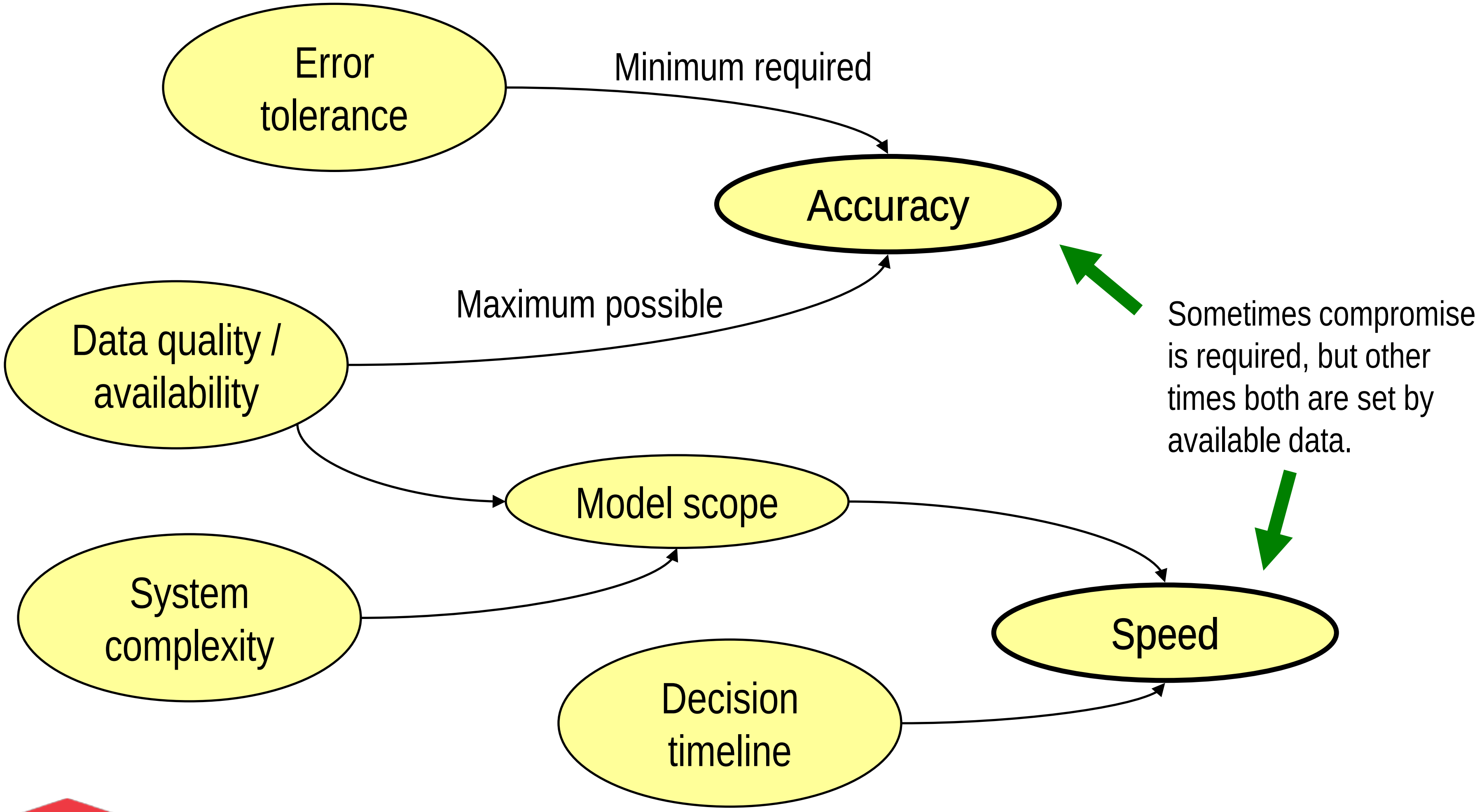
Are we modeling the right things to meet the business needs?

Are we generating data accurate enough to make the correct decisions?

Are we generating data fast enough to make decisions when needed?

Some trade-off, but not always

Accuracy vs. Speed – Real Life is Messy!



The key to success for the Execution phase is Project Management

Everything is a project

Hence everything needs good project management skills

The Definition phase is the First Step in successful project management

You just did this so you are already on the right track!

Invest in yourself and your team – upgrade the PM skill sets

Simulation as Our "Product" via the Six Sigma DMEDI approach

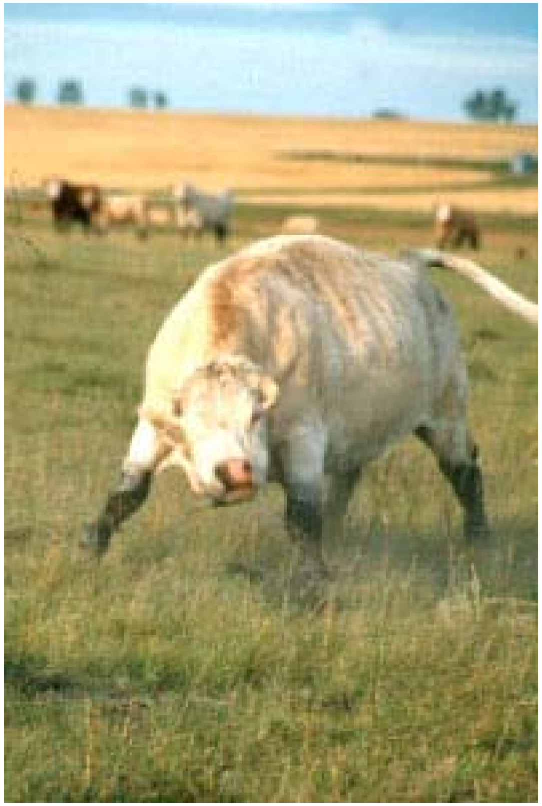
Define	Define the project using the project charter (scope, deliverables)
Measure	Measure VOC data, translate to Critical to Customer Requirements (model metrics and variables, functionality specifications, accuracy, speed)
Explore	Explore conceptual model designs (theory, solution algorithm, software applications, user interface features)
Develop	Develop the detailed model design and verify via prototyping (computer model)
Implement	Implement the model to support decision making, optionally hand over model to customer

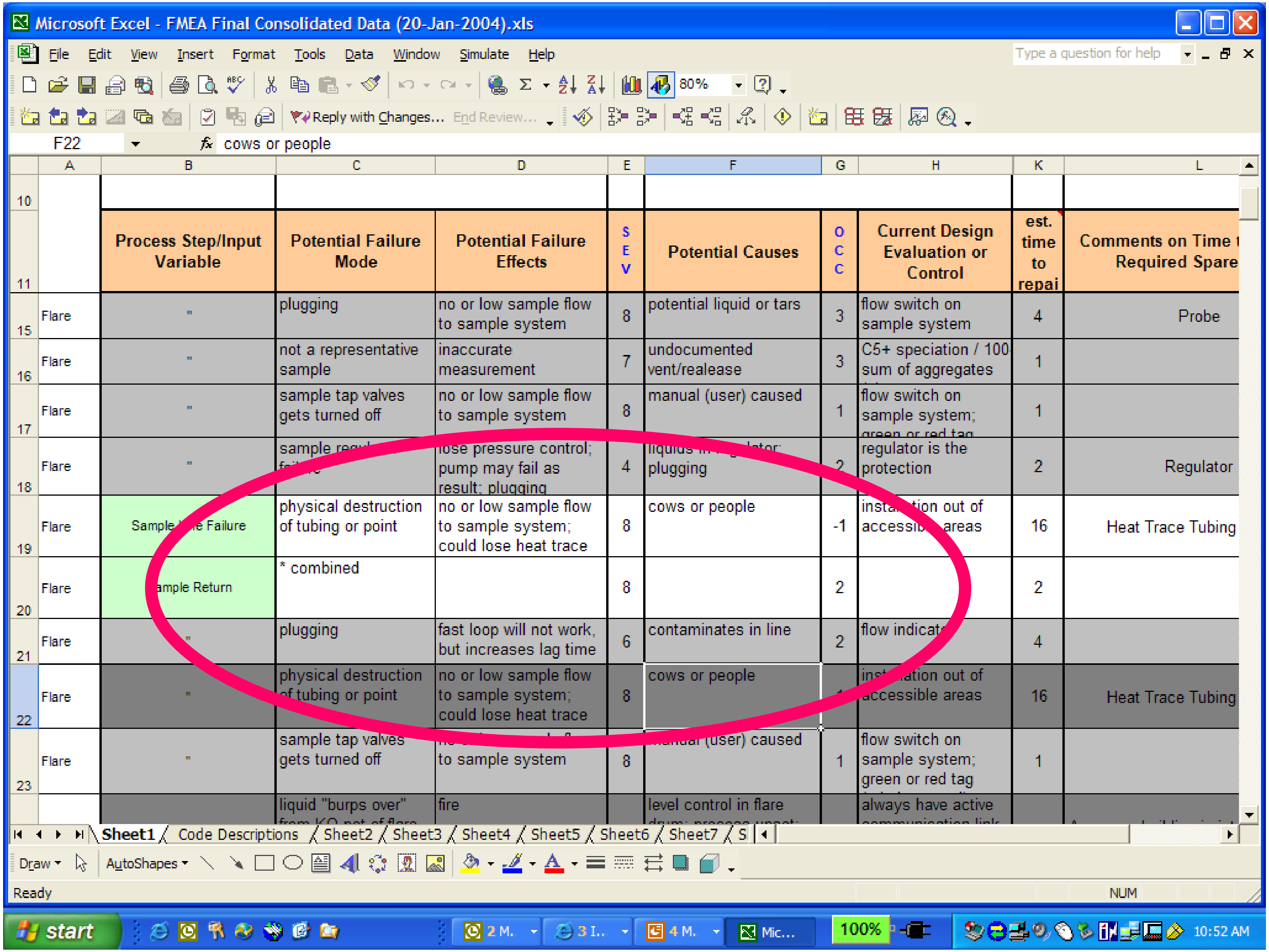
DOW®

Concluding Remarks

- For industrial problem solving, how we do simulation is dictated by the decision making that we support.
- We need to get answers quickly and efficiently, even if the system is complex. We don't want to model anything and everything. We are also not interested in a perfect solution of a toy problem.
- Our current focus is efficient techniques that support rapid decision making under risk.
- Development of methodologies combining simulation and other techniques is a research area of practical importance.

And sometimes you have simulate cows…




Microsoft Excel - FMEA Final Consolidated Data (20-Jan-2004).xls

F22 cows or people

Row	A	Process Step/Input Variable	Potential Failure Mode	Potential Failure Effects	SEV	Potential Causes	OCC	Current Design Evaluation or Control	est. time to repai	Comments on Time t Required Spare
15	Flare	"	plugging	no or low sample flow to sample system	8	potential liquid or tars	3	flow switch on sample system	4	Probe
16	Flare	"	not a representative sample	inaccurate measurement	7	undocumented vent/realease	3	C5+ speciation / 100 sum of aggregates	1	
17	Flare	"	sample tap valves gets turned off	no or low sample flow to sample system	8	manual (user) caused	1	flow switch on sample system; green or red tag	1	
18	Flare	"	sample regul[illegible]	lose pressure control; pump may fail as result; plugging	4	liquids in [illegible] plugging	2	regulator is the protection	2	Regulator
19	Flare	Sample [illegible] Failure	physical destruction of tubing or point	no or low sample flow to sample system; could lose heat trace	8	cows or people	-1	insta[illegible]tion out of accessib[illegible] areas	16	Heat Trace Tubing
20	Flare	[illegible]ample Return	* combined		8		2		2	
21	Flare	"	plugging	fast loop will not work, but increases lag time	6	contaminates in line	2	flow indicat[illegible]	4	
22	Flare	"	physical destruction of tubing or point	no or low sample flow to sample system; could lose heat trace	8	cows or people	[illegible]	inst[illegible]ation out of accessible areas	16	Heat Trace Tubing
23	Flare	"	sample tap valves gets turned off	[illegible] to sample system	8	[illegible] (user) caused	1	flow switch on sample system; green or red tag	1	
			liquid "burps over"	fire		level control in flare		always have active		

Sheet1 / Code Descriptions / Sheet2 / Sheet3 / Sheet4 / Sheet5 / Sheet6 / Sheet7

Might have been a good Agent-based simulation