HTR Informatics

DOW

Issues and Challenges in the Management of Data and Knowledge from High Throughput Research in Catalysis and Material Science

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HTR at Dow Chemical

- High Throughput Research is a ***HOW*** not a ***WHAT***
- High Throughput Research can be applied to any of Dow's product lines and processes
  - Homogeneous catalysis processes
  - Heterogeneous catalysis processes
  - Polymers (thermoforms & thermosets)
  - Formulated products
  - Agrochemicals
- Focus is often on the process, not the product, except that the process often defines the product
- High project turnover

Discovery vs. Process Research

Discovery Research

- Screening
- Yes or No tests
- Look for an event
- # samples large
- Sample size small
- # condition sets small

Process Research

- Optimization (multi-valued)
- Mixtures
- Measurement precision
- # samples small
- Data complex
- Sample size larger
- # condition sets larger
- Data integration
  - With other reactors
  - Across scales

Example Project: Catalyst Modifier

- **Problem:** Polymer product; small amounts of a side product coat reactor over time
- **Task**: Modify the catalyst package and process conditions to eliminate the side product
- Resulting data
  - Structures & amounts of catalyst modifiers (~300 candidates)
  - Reactor conditions (Temperatures, pressures, flows versus time)
  - Analytical results (GPC, DSC, FTIR)
  - 3 months work; ~50 boxes of paper (if printed)
- Solution was a *combination* of process changes and a catalyst modifier

Informatics

- Conducting experiments is no longer the bottleneck
- It can often take longer to collate the pertinent synthesis, reaction and screening data that it does to run the experiments
- Multiple screens required for multivariable optimizations
- Still have people who prefer a week in the laboratory to an hour in the library

Challenges for Informatics

- Complex experiments
- Complex data
- Need data about how the experiments were executed (i.e. process variables)
- Dynamic workflow
- High project turnover (~100/year)
- Multi-variable optimization problems

Big Challenge #1

Can We Afford the High-Tech Solution?

Big Challenge #2

Can’t just cut open the shrinkwrap

Addressing the Challenges

- Leverage what we can from pharmaceutical industry experience
- Define a flexible architecture
- Use an agile methodology
- Communicate, communicate, communicate

Informatics Architecture Principles

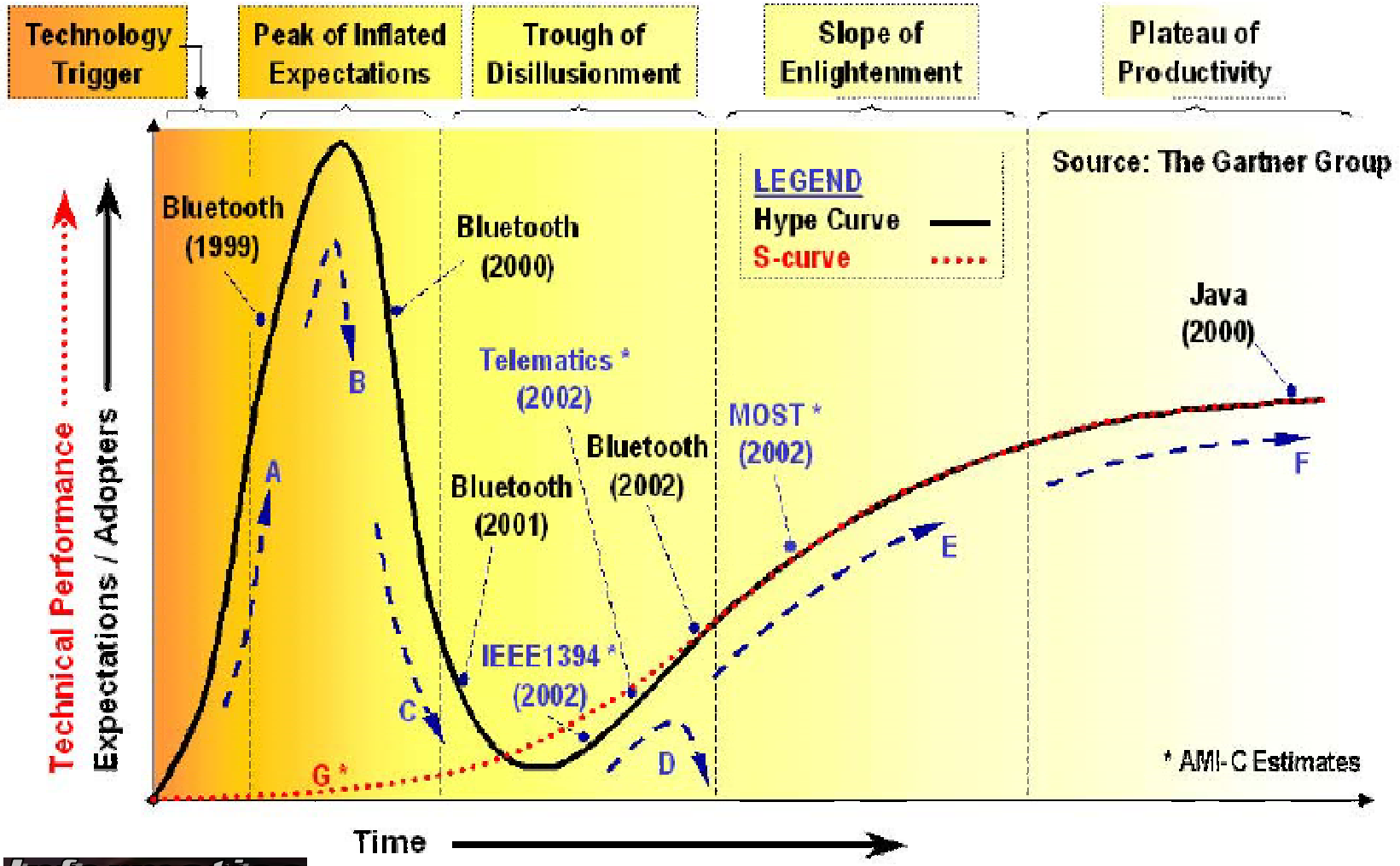
- Use purchased software where practical
  - Understand want versus need
  - When can the workflow adapt to the solution
  - When must solution adapt to the workflow
- Design for the long term (possible 75 year retention)
  - Use published data formats
  - Keep data migration paths in mind at all times
  - Underlying applications will change
  - Maintenance dominates total cost of ownership
- Applications which must be “in charge” are bad
  - Must be able to talk with other applications
  - Use Web Services as application glue

Agile Development

- Lots of Agile Methods: XP, Orange, Crystal, Scrum, …
- Studied available methodologies, chose something of a hybrid
- Short inspect and adapt cycles
- Focus on delivering something usable by the customer
- Understand the cost of changes
  - Build now, refactor later
  - Getting something useful now helps drive out requirements

Communications

Stages of the Hype Cycle



Summary

- Wetware is at least as important as hardware and software
- Architecture and implementation methodology are at least as important as the tools
- “Center of the universe” applications and tools are bad