Engaging Scientists in the Adoption of Automation

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Why?
• Why Automation?
• What is Effective Automation?
• Importance of Equipment Evaluation
• Automation at AZ
  • Range of Approaches
  • Range of Equipment
  • Range of Users.
  • Automation Adoption.
Why?

Increase productivity
Enabling unattended operation
Increase throughput
Minimising human intervention
Produce higher quality data
Obtain a greater density data
And much more ……….
What is Effective Automation.
Importance of Equipment Evaluation

- Understand costs vs benefits
- Resource required
- Engage end users
- Support change management
- Define specific configuration
- Compare alternatives
- Use real-case examples
  - Chemistries / processes
  - User groups
Can we automate a process from start to finish on one platform?
To evaluate the possibility to investigate process from start to end
- Weighing / Work-up / Filtration
- Use project examples
- Investigate a number of experimental variables, using a statistically designed set of experiments
Fully Automated?

Conversion (%)

Time (hr)

Conversion (%) vs. Time (hr) graph

Fully Automated? Flowchart:
- Scale
- Beaker
- N₂
- Scale
- Thermometer
- Clock
Planning and Design
Statistical or Kinetic

Reaction Preparation
Solid Handling

Liquid Addition and Reaction

Analysis
HPLC GC UPLC

Interpretation
Analytical data

Conclusions
Reporting

Semi – Automated Workflow
Would chemists carry out a number of experiments in parallel if it was as easy as carrying out one?
Do we want to carry out more experiments in parallel or collect more data from each experiment?

• To investigate using Automated Lab Reactors (EasyMax/OptiMax) and associated software to automate part of the process of experimental write up and data capture.

• LabConnect Trial on AZ project to:
  • Evaluate the ability of scientists to use the EasyMax as a personal reactor to carry out all chemical operations.
  • To enable effective re-use of experimental details and data.
  • To work with vendor and other companies to direct and exploit the development of the software.
  • Engage scientists to help devise a fit for purpose solution.
Increase in the number of parallel reactions?
Data/information from each reaction

Number of reactions

Specialist

Flow
Screening
FED / DoE

Generalist

Crystallisation
PAT
Scale-Up
Data/information from each reaction

Number of reactions
Automation Uptake

- Asymmetric H2
- TM-catalysis

Why?

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