

ACCELRY'S EXPERIMENT KNOWLEDGE BASE (EKB)

The Experiment Knowledge Base is a Packaged Professional Services solution that helps scientists to develop new, better materials through more efficient and more effective experimentation. Part of the Accelrys Enterprise Lab Management suite designed to support all aspects laboratory operations, EKB adds capabilities for planning and execution of experiments, as well as managing, mining and analyzing experimental data to the Pipeline Pilot enterprise informatics platform.

The diversity and complexity of the modern materials laboratory makes it difficult to transform scientific *data* into *knowledge* that informs decisions. Because of this, up to 40% of all experiments run are actually repeats of work that's been done before but can't be found or evaluated. EKB improves laboratory efficiency & productivity, accelerates time to innovation and supports Sustainability strategies by improving:

- **Experiment Planning** – knowledge-driven and statistically designed experiments to minimize cost and maximize effectiveness in the lab.
- **Experiment Execution** – tracks workflow, gathers data produced from instrument files, spreadsheets and databases and eliminates manual piecing together of data.
- **Data Analysis** – powerful queries and visualization of experimental results.
- **Reporting** – Configurable report templates with integrated charting, scatter plots and interactive reporting options.

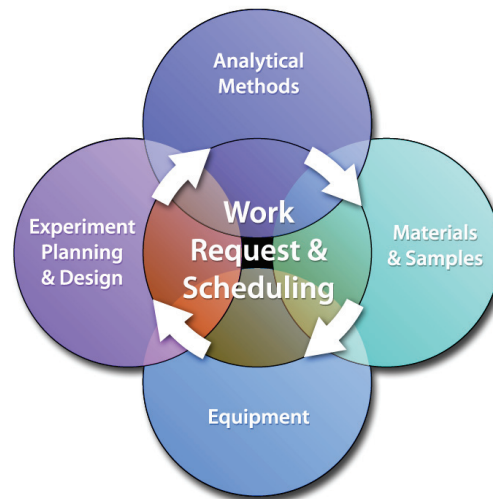


Figure 1: Accelrys Enterprise Lab Management Suite

- **Data Mining and Knowledge Generation** – Builds correlative and predictive models to compare data across R&D scales (screening, bench-scale, pilot units) and provides statistical guidance on what experiments should be performed next.

MORE VALUE FROM LABORATORY DATA

Most laboratories engaged in researching and developing chemically-based materials have a variety of instruments and systems in place that create and “manage” experimental data with varying degrees of effectiveness. This complex information environment makes it very difficult to establish the trends, patterns and relationships between experiments and their results that make the data valuable to store in the first place – leaving scientists unable to answer basic questions such as:

- “What experiments have I already run using materials in this concentration, under these conditions?”
- “What do the results tell us? How do they compare to other similar experiments?”
- “What experiments should I run next to answer my questions and achieve my goals?”

Even with LIMS and other laboratory data management systems in place, scientists struggle to find and interpret information from previous experiments. This inability to learn from previous efforts causes up to 40% of all experiments to be repeated needlessly, wasting resources, time, and money.

EKB works with existing laboratory systems and equipment to extract raw experiment data and add material descriptors to enable sophisticated querying and mining that shows trends and patterns to inform scientific decision making as well as further experiment planning.

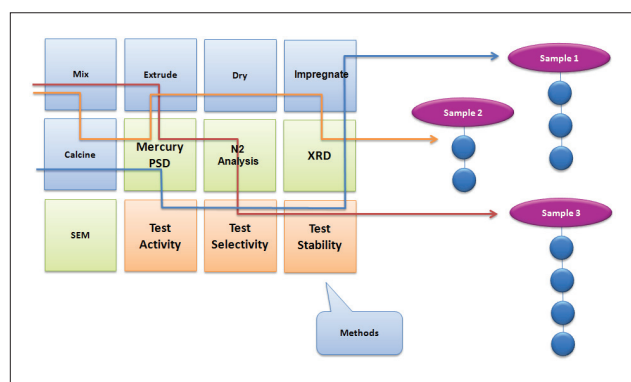


Figure 2: Material workflow.

EXPERIMENT PLANNING & DESIGN

Using EKB, scientists can create new experiment plans or derive them from templates of previous experiments. EKB supports definition of experiment workflow (sequence of processes), input parameters for processes and the number and origin of the samples that will pass through the workflow.

To answer questions and develop materials quickly and efficiently, it is critical that the number of samples and therefore overall cost of experimentation is minimized. EKB supports ad-hoc experiment planning as well as statistical “Design of Experiments” (DoE) tools that help scientists design experiments efficiently; combined with the ability to find and reuse the results of previous experiments EKB enables planning and design of new experiments that have maximum impact with minimum cost.

MANAGING EXPERIMENT EXECUTION

EKB provides a “plug-in” system that enables direct integration of experiment plans with existing laboratory equipment and systems. Equipment operators receive clear and consistent instructions within experiment plans and otherwise work with instrumentation exactly as they do today. EKB’s experiment dashboard shows progress of all samples in the experiment plan.

Experiment data is uploaded to EKB via direct import from instrument files, from a database, or through manual upload. Scientists can leverage Pipeline Pilot capabilities to create “validation

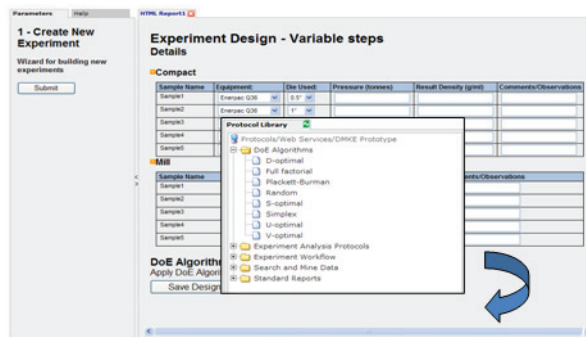


Figure 3: Experiment Planning Wizard.

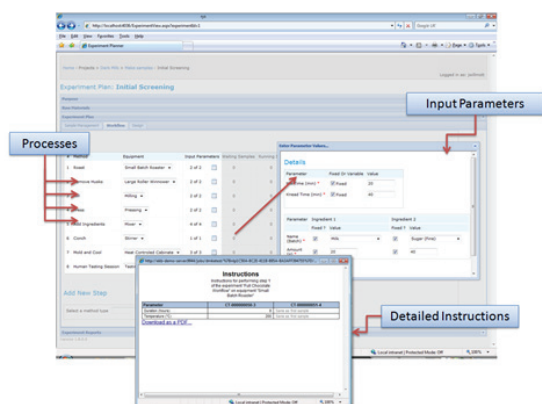


Figure 4: Step by Step Guide to Experiment Execution.

wizards” that take users through a sequence of visualizations of recently uploaded data designed to help them determine if the process has worked and the data is correct. Visualizations typically include line plots, scatter plots and tables that help to improve data quality and consistency in experiment execution.

SAMPLE PEDIGREE

Materials research commonly involves dividing original material samples into subsamples whose pedigree or history is important to a scientist's understanding of experiments and the relationships between sample properties. EKB captures sample pedigree in terms of the sample's parent, children and siblings, and other materials that have been combined (mixed) with the sample during processes.

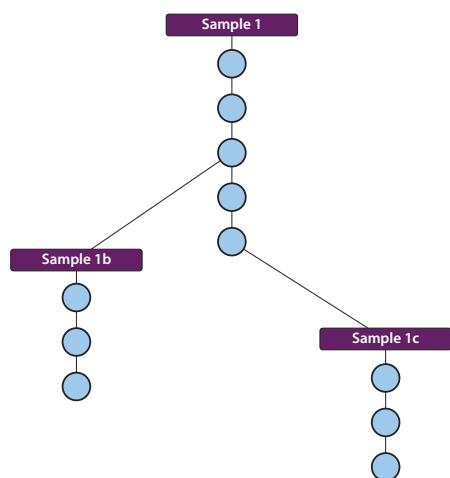


Figure 5: Sample Pedigree.

ANALYSIS OF EXPERIMENT DATA

EKB provides extensible capability to find, analyze and visualize experimental data using the power of the Pipeline Pilot informatics platform. The system features a highly flexible search engine based on material descriptors for all the samples in the database. Categories of descriptors available for single or multi-criteria search include but are not limited to:

- Input Parameters
- Output Data
- Sample Pedigree (parent, siblings, children, raw materials, reagent batches used)
- Sample Origin (who made it, which project)
- Workflow (sequence, number of times through a process)

EKB provides comprehensive tools to visualize experiment data, including tables, histograms, scatter plots and more. Plug-in capabilities also enable integration with 3rd party analysis tools such as Microsoft Excel™ and Spotfire™.

EKB also supports statistical data mining, enabling scientists to spot trends and patterns that speed the materials innovation process. Examples include principle components analysis (correlations between parameters), factor analysis (correlations between parameters), cluster Analysis (sample groupings) and predictive models (statistically generated suggestions on “next best lead”).

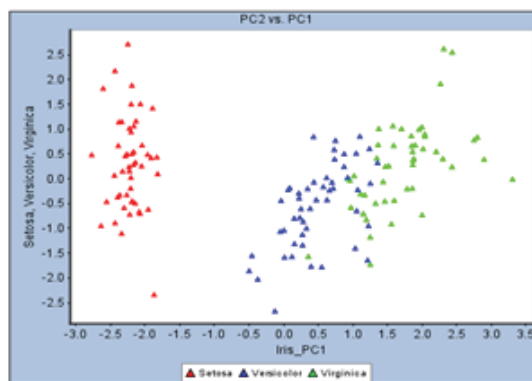


Figure 6: Data Analysis & Visualization.

EMPOWERING SUSTAINABILITY

Benefits of EKB include improved laboratory efficiency & productivity, faster time to innovation and scientific/laboratory operations that support customers' Sustainability strategies. These benefits are delivered through:

- Extraction and collection of descriptive information from multiple data sources such as LIMS, Excel, and databases
- Better, more informed experiment plans
- Faster experiment execution
- Faster analysis of experimental data
- Fewer repeat experiments
- More scientific insight and value from all experimental data

IMPLEMENTING EKB AT YOUR ORGANIZATION

The Accelrys Experiment Knowledge Base is available as a packaged solution from the Accelrys Solutions Consulting team.

To learn more about Accelrys Experiment Knowledge Base, go to accelrys.com/ekb