Chemicals & Petrochemicals
Analytical solutions in the laboratory

Intelligent Workflow for High Throughput Routine Analysis

The correct composition of medical cleaning solutions is extremely important and must be rigorously tested. For Dr. Weigert GmbH, a fully automated, multiparameter system from METTLER TOLEDO performs all the required analysis, including automated method selection, secure data handling and even solution waste management.

Dr. Weigert GmbH, a German chemical producer based in Hamburg, manufactures cleaning solutions used for cleaning and disinfecting medical instruments. The composition and quality parameters of such solutions are extremely important and must be rigorously tested. Due to the high demands of these solutions, and a responsibility to their customers, Dr. Weigert was looking for an automated system to speed up their multiparameter analyses.

A modern, multiparameter system
With a high sample throughput, the QC lab at Dr Weigert needed a modern, fully automated system to perform multiparameter analysis with automated method selection for each sample. Depending on the sample requirements, density, refractive index, acid/base number, active chlorine content and pH can be determined. METTLER TOLEDO devised a system that performs all the required analysis followed by automated cleaning, conditioning and waste management. The system also ensures secure data handling.

A DM40 density meter connected to LabX® PC software lies at the heart of the system. The density meter is connected to an Excellence T90 titrator, a RX50 refractive index cell and a SC30 automation unit fitted with a barcode reader. Samples are labelled with a 2D barcode on the vial and placed on the SC30, which reads the data. The SmartCodes™ functionality in LabX automatically selects the correct analysis method for the sample.
Due to the high alkalinity of the chemicals measured, contact with the density measuring-cell must be kept to a minimum to avoid damaging the glass. The system ensures that the density cell is thoroughly rinsed as soon as the measurement has finished. Due to the differing chemical properties of the samples, the automated system ensures that waste solutions are separated and stored accordingly.

All data is stored by LabX software and analytical results are automatically transferred to a LIMS system where a plausibility check decides if results fall within specification. A task scheduler is also predefined in LabX to enable system conditioning and preparation to be performed at the start of the day. In this way, the system is ready for the first sample when the first operator arrives in the lab.

**Fully automated and secure workflow**

The multiparameter system provides a fully automated and secure workflow that includes pre-analysis conditioning, method selection, cleaning, waste management and data handling. Productivity is increased, transcription errors eliminated and operator time kept to a minimum. All the operator has to do is press the ‘SmartCode Start’ button on the master, density meter interface and place new samples on the automation unit. This means an easy, safe and very efficient quality control system for Dr. Weigert.

Text: Daniel Buchmann  
Density & Refractometry Product Manager

Enzymes are catalysts that enhance the rate at which biologically relevant chemical reactions occur. There is, therefore, a substantial interest in ‘designing’ enzymes to perform non-biological catalysis.

In the paper, “Precision is essential for efficient catalysis in an evolved Kemp elimination,” a team from Caltech, The University of Zurich and ETH Zurich optimized the non-biological enzymatic reaction catalyzed by a designed enzyme named HG3. By using 17 rounds of PCR and DNA shuffling, the team was able to increase the efficiency at which HG3 carried out a Kemp elimination reaction by over 500-fold. This brings the team very close to the rates observed in chemical reactions catalyzed by natural enzymes.

The experiments required a number of enzyme variants to be generated and screened. In order to generate the required enzyme variants, the researchers grew bacterial cultures in 96-well plates. After the induction of enzyme production, the cells were grown and enzyme activity was measured using the intact cells. In order to re-suspend the cells before the enzyme assay, the team used METTLER TOLEDO Liquidator 96 to rapidly mix the suspension to uniformity.

Enzymes play an important role in the catalysis of chemical reactions and dramatically speed up reaction times. Researchers have succeeded in ‘designing’ an enzyme able to perform non-biological catalysis, an important breakthrough with multiple applications.

The Liquidator 96 assists in sensitive cell-based methods in addition to proteomics and genomics protocols. With simultaneous, 96-channel pipetting, it is impossible to skip wells or pipette twice into the same well. Liquidator 96 also greatly speeds up this process by filling a 96-well plate in just 6 seconds.

Text: Rishi Porecha
Rainin Application Specialist

www.mt.com/liq96

Read the paper published in “Nature”
Moisture Analyzer
Speeds up QC of Concrete Accelerator

Sprayed concrete is an integral part of solid rock support systems for mines, tunnels and other civil engineering structures. UK-based Normet, which produces sprayed concrete and other chemical supports for tough engineering projects, needed to reduce the time required to dry quality-control samples of its specialized injectable Tamshot 80 AF additive.

TamShot 80 AF (Alkali-Free) is used for wet mix 'shotcrete' processes in tunneling and mining. It is applied where initial rock support is needed or a permanent lining has been designed. The high-performance quick-setting liquid additive can reduce concrete setting times without risking a caustic work environment thanks to its low alkali content (<1%).

Queuing at quality control
The high demand for their products, combined with the extensive drying time required for the oven-drying methods Normet relied on, meant that products were often sitting waiting for quality control results before they could be dispatched.

Droplets of Tamshot80 AF are spread evenly on a glass-fiber filter to ensure uniform drying with the HB43-S
This led David Galloway, one of the company’s UK-based quality-control chemists, to check into the possibility of using a halogen moisture analyzer. With the help of his local METTLER TOLEDO representative, he chose the HB43-S.

**Developing a workable method**

HB43-S is ideal for monitoring the moisture content of a substance such as TamShot. The halogen drying technology significantly reduces sample drying times and minimizes workload for testing operators. However, to meet regulations, the results from the HB43-S had to be cross-validated against Normet’s oven-drying reference method which stipulated that TamShot be placed in the oven for 4 hours at a temperature of 105°C.

HB43-S held the promise of delivering results similar to the drying oven in about 15 minutes at slightly higher temperatures. However, developing the correct parameters for measurements using the moisture analyzer can require several tests. Mr. Galloway contacted METTLER TOLEDO product manager Claas Boerger to see if, together, they could come up with a method that would match the necessary reference values while simultaneously speeding up the entire process.

**A successful partnership**

Mr. Galloway sent Mr. Boerger enough TamShot to perform several tests against the reference method. After the test sessions, the ultimate solution was developed. Normet now uses a glass-fiber filter that speeds up measurement time and improves measurement accuracy by increasing the surface and enabling better evaporation. Additionally, TamShot was applied to the filter using a dropper to ensure even application and prevent it from rolling up and touching internal surfaces of the analyzer (which can negatively affect results).

Today, Normet has drastically speeded up quality control with a method to determine moisture content that takes an average of 14 minutes per test. This is a significant reduction from the previous 4 hours and all results remain within an acceptable standard deviation of 0.49%. All told, Normet is able to test TamShot 80 AF much more quickly while obtaining the kind of results that keep the popular product strong, reliable and sought-after.

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Text: Claas Boerger  
Moisture Analyzer Product Manager  
www.mt.com/moisture
Understanding Thermal Risks
to Create Safer Chemical Processes

Most chemical processes are carried out in batch or semi-batch mode where hazard potentials and process risks are related to chemical reactivity, reagent toxicity and process design. While reagent toxicity cannot be influenced, appropriate process design can keep reactions under control. This is possible only through obtaining a complete understanding of process dynamics.

Thermal process dynamics take on a special meaning in batch and semi-batch chemical processing where they have the ability to produce runaway scenarios. These scenarios are ultimately related to conditions in which the heat generation of an ongoing reaction exceeds dissipation capacity. The causes of this range from reactant accumulation during cooling failure to wrong kinetic assumptions in process design. Reactant accumulation, sensitivity to impurities and reaction initiation problems can also promote runaway.

Even very weak reactions can runaway under the right conditions. For these reasons, it is critical to gain a complete understanding of reaction dynamics to help determine process criticality and risk. This is of particular importance when preparing for scale-up as potential loss of product or even life is at stake.
Understanding reaction maximums

Gathering calorimetry and heat flow data to predict reaction progress is easily achievable. This can help to reduce or even eliminate runaway potential. As it is not feasible to completely model the reaction in practice, analyses can be effectively reduced to certain basic properties. A ‘runaway graph’ can be developed from these properties to give information concerning process design.

Essential questions asked include: What is the heat evolution rate as a function of time? At what temperature will runaway occur? When is reaction temperature maximal? Can a decomposition reaction develop? What is the order of magnitude of an adiabatic temperature increase caused by secondary reactions? And, of course, what are the consequences?

Obtaining data

One of the most appropriate tools for modeling reactions under representative process conditions is METTLER TOLEDO’s Reaction Calorimeter RC1e®. Automatic heat-flow measurement indicates reaction rate. Reactant accumulation is calculated from conversion as a time function while energy accumulation is obtained by integrating the heat flow curve.

Subsequent micro-thermal analysis of starting materials and intermediate samples using a method, such as differential scanning calorimetry (DSC), helps determine desired and undesired reaction signals. Heat evolution of secondary reactions and physical property characteristics are also gathered.

Evaluating criticality

Process risk depends upon the severity and probability of occurrence. Thus, runaway criticality can be evaluated using relative temperature levels and any decomposition reactions proceed under adiabatic conditions. Probability is then estimated on a time scale. If emergency concerns and measures can be taken before runaway becomes too fast, runaway probability remains low.

Text: Urs Groth
AutoChem Product Manager

www.mt.com/chemical-safety
Anne Swapped her Journal for LabX
Be Next in Automating Your Workflow

Anne is a Laboratory Manager whose lab performs a wide variety of analyses, mostly for quality control purposes. Recently, Anne was tasked with finding a way to automate these analyses, optimize operators’ time and ensure traceability and compliance with the rising regulations.

Anne concluded that the key needs were related to integration, either of instruments, systems, or reports, and automation of analyses, workflows, and data. She decided to adopt LabX in her laboratory to address these challenges.

Today, her instruments are connected, methods started with just one click and lab journals replaced with a secure database.
Smooth, error-free workflow
On the instrument, step by step guidance directs the operator. All work is ensured to be in accordance with internal SOPs.

Full data management
All information is automatically stored in a secure database to ensure traceability. See, store or print results in a customized report at any time.

Tailored set up
Develop and implement SOP compliant application methods ready for use on the relevant instrument. Define the roles of individual users and set-up the daily task list.

Power Your Bench with LabX® Software

Instrument connectivity
LabX connects Mettler Toledo instruments to a single software. A unique interface means less training and more efficiency.

Learn more about LabX
www.mt.com/LabX
Automatic and Highly Accurate Melting Point Determination

The MP50 Excellence performs automatic determination of melting point and melting range up to 300 °C, measuring up to four samples simultaneously. Outstanding temperature-accuracy specifications ensure accurate measurements and the whole melting process is video recorded and can be played back any time on the instrument.

Superior Usability
The large color touch screen with One Click® shortcuts is quick to learn and easy to operate. Twelve different melting point determination methods can be set up and started via shortcuts.

Trustworthy measurements
Highly accurate melting point and melting range temperatures are obtained with the automatic measurement of transmission intensity. The intensity curve can be viewed at any time – during measurement or while reviewing the results.

Never Miss a Melting Point
For unattended measurements, visual data is stored on the instrument. The high resolution video-recordings of the melting process can be replayed at any time at the instrument or at the computer.

www.mt.com/MP50
Put Your Lab InMotion™ for Flexible and Efficient Analyses

Automation in today’s laboratory has high demands for a variety of samples and workflows. Automation no longer means just analyzing one sample after another. Autosamplers assist with making workflows more flexible and efficient by eliminating process orders and sample data transcription errors.

Maximum throughput
Designed to maximize throughput in the minimum of space, InMotion autosamplers increase productivity without sacrificing laboratory bench space. The innovative robotic arms of the Pro and Max series reach into the sample tray to optimize space.

Flexible workflows
Intuitive and flexible instrument programming allows sample workflows to be tailored to specific requirements. Whether using PowerShower™ to clean components or more thorough sequences to clean and recharge electrodes, In-Motion is here to assist.

Modular and tailored
Every lab and sample has its own demands. Build an autosampler according to sample requirements with modular boards for extra pumps, CoverUp™ system for protecting samples and operators and water bath sample trays for temperature control.
Know-How

Straightforward Routine Testing
Minimize Risks and Costs

Testing laboratory instruments periodically is not only a way of complying with regulations but also the key to obtaining accurate and reproducible results.

Routine testing can be, however, a tedious and complex task. Our whitepapers provide you with recommendations about when and how to perform a routine testing on your instruments – among other good practice tips!

Step-by-step guidance for eased instrument routine testing

Balances
www.mt.com/RT-balances

Pipettes
www.mt.com/RT-pipettes

Moisture Analyzers
www.mt.com/RT-moisture