Direct sample analysis combined with a thermal gradient approach for routine testing of materials

Cristian Cojocariu
Waters Scientific Operations
Analytical challenges in Materials Testing Laboratories

1. Cost-efficient, fast analysis time from ‘sample to knowledge’

2. Robust, reliable analytical measurement

3. Quick result (pass/fail) from batch to batch

4. Minimal or no sample preparation (liquid or solids); reduce or eliminate the use of hazardous solvents
What is RADIANT ASAP?

Rapid Direct Analysis – Atmospheric pressure Solids Analysis Probe

- A novel, dedicated direct mass analysis system, engineered using proven and robust technologies
- Specifically designed for rapid, easy and low cost per sample analysis of solids and liquids.
- State of the art informatics tools to enable easy, real time results
Key features of RADIAN ASAP

- **Suitable for a wide range of samples**
  - High to low polarity analytes
  - Volatile and semi-volatile solids, liquids, and solutions

- **Simple analysis workflow**
  - Minimal to no sample preparation
  - Minimal training required
  - Open to use by non-expert personnel

- **Real time results for Raw Material & Formulation analysis**
  - LiveID & IonLynx software for real-time sample identification library matching compositional analysis

- **Fast**
  - Minimal time from sampling to result

- **Small footprint**
  - Make the most of available lab space
    - W:34.4 cm/13.5", H 27.1 cm/10.7", D:73.0 cm/28.7"
How does RADIAN ASAP work?

Analysis in four easy steps

1. Clean the capillary
2. Load sample on capillary
3. Insert capillary to start acquisition
4. Real-time data visualization
How does RADIAN ASAP work?

The ASAP ionization process

- Sample is introduced into the corona discharge region on a glass rod
- Volatilised by stream of heated N₂
- Gaseous analyte molecules are ionised by N₂ plasma
- Gaseous ions are guided into the instrument and analysed by the single quadrupole analyser

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**ASAP – The mechanism of ionization**

### Charge Transfer
- Favoured by relatively non-polar compounds

### Proton Transfer
- With presence of protic solvents such as H₂O or MeOH
- Favoured by relatively polar compounds

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Example applications: Raw Materials Authenticity
Raw Material Authenticity

- Chemical Industry:
  - Incoming raw materials need to be verified
  - Out of specification or contaminated substances need to be investigated
  - The quality of formulated products needs to be confirmed

- Decreasing the time to generate data on which decisions are made is key

- Reduction in analysis time allows laboratories to increase productivity and deliver results efficiently
Quality Control Laboratories are responsible for ensuring all received raw materials conform to specification.

QC Scientists utilize a range of analytical techniques to confirm the ID and purity of raw materials prior to formulation.

Formulation Scientists design, prepare and test the formulations in iterative processes to develop new and improved products.

Finished products are passed back to QC Scientists to perform batch release tests before release to market.
Chemical Manufacturing Workflow – Current Analytical Technologies

Receive Raw Materials

Verify Raw Materials

Formulate

Verify Formulation Batch QC testing

Identity & Purity Tests

In Process Monitoring Prototype performance testing

Batch Release Testing

FTIR / UV Spec: time consuming sample prep, ambiguous results, no mass info

PAT: expensive to implement, requires expert operators

Batch Release Testing: Requires specialist operators

RADIAN ASAP: fast, rich mass spectral data for rapid decision making

FTIR / UV Spec: time consuming sample prep, ambiguous results, no mass info

LC / GC-MS: expensive, long analysis time, long queue

Performance testing: can require expensive bespoke equipment

Physical Property Measurements: Requires specialist operators

RADIAN ASAP: fast, rich mass spectral data for rapid decision making

The above text describes the chemical manufacturing workflow, emphasizing the challenges associated with current analytical technologies. Key points include:

- **Receive Raw Materials**: This stage involves verifying the identity and purity of raw materials.
- **Verify Raw Materials**: Further steps are taken to ensure the materials meet the required standards.
- **Formulate**: The process of formulating the materials into the final product.
- **Verify Formulation Batch QC testing**: Quality control checks are performed on the batch to ensure it meets specifications.

**Current Analytical Technologies**

- **FTIR / UV Spec**: Time-consuming sample preparation, ambiguous results, no mass information.
- **MT**: Cheap, laborious, time-consuming, operator variability.
- **LC / GC-MS**: Expensive, long analysis time, long queue.

**Identity & Purity Tests**

- **In Process Monitoring**: Prototype performance testing.
- **Batch Release Testing**: Expensive to implement, requires expert operators.

**Physical Property Measurements**

- Requires specialist operators.

**RADIANT ASAP**: Fast, rich mass spectral data for rapid decision making.
Temperature ramping as a tool for separation

- Temperature ramp separates compounds based upon boiling point
- Different spectra at different temperatures
- Basic deconvolution of complex samples

PEG 600 polymer + four additives
Rapid Analysis of Raw Polymeric Materials

PEG 600 polymer + four additives

Higher mass oligomers (low intensity)

Lower mass oligomers

Middle mass oligomers

Higher mass oligomers

Cyasorb 2908

Octabenzene

Irgafos 168

Oxidized Irgafos 168

Irganox 1010

Cyasorb 2908

Octabenzene

Irgafos 168

Oxidized Irgafos 168

Irganox 1010
Example applications: Face masks analysis
Manufactured Mask Sample

TIC for the white part, the blue part, and both parts together in positive ion mode

Mask intact: blue & white fragments

Blue mask fragment

White mask fragment
Results & Discussion: Manufactured Mask Sample

Example spectra at different time/temperature points for the white fragment in positive ion mode.

- Oxidized Irgafos 168
  - M = 646.45
  - [M+H]^+ = 647.45

- Dibutyl phthalate
  - M = 278.15
  - [M+H]^+ = 279.16

- PP Irgafos 168
  - M = 662.45
  - [M+H]^+ = 663.45

- CH₃
- CH₂CH₃

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Results & Discussion: Manufactured Mask Sample

Example spectra at different time/temperature points for the blue fragment in positive ion mode

![Irganox 1010 spectra](image)

\[ \text{M} = 1176.78 \]
\[ (\text{M}^+ = 1176.78) \]
\[ [\text{M+H}]^+ = 1177.79 \]
Summary

- Compact, easy to use direct sampling mass detector
- Minimal need for training and system preparation, suitable for non-MS experts
- Rich mass spectral data obtained in as little as 30 seconds enables rapid decision making and increased workflow efficiency