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Nota applicativa

Providing Quick and Easy Quality Control to the Polymer Industry Using the SQ Detector 2

Waters Corporation



This is an Application Brief and does not contain a detailed Experimental section.

Abstract

This application brief demonstrates the utility of an SQ Detector 2 for clear and simple Quality Control (QC) monitoring of polymer additive blends, and to rapidly identify out of specification batches.

Benefits

The SQ Detector 2 was used to help identify two different types of formulation error quickly and easily.

Introduction

In the polymer industry, materials developers and manufacturers face on-going challenges to reduce costs, improve return on investment (ROI), and enhance product performance. Errors in batch blending or product formulation could prove extremely costly, both financially, if a manufacturing process needs to be stopped, and in reputation, if substandard products are supplied to customers. Consequently, QC monitoring of raw materials and final products are of vital importance.

QC testing activities need to be quick and easy to interpret to ensure the minimum delay between testing and providing feedback to the production line – especially if a faulty batch has been detected. In some cases, the tested batch may need to be withdrawn, which has a significant cost implication. Alternatively, a blending error may be benign and the batch can be used in its supplied formulation, providing valuable savings to the company.

A simple visual observation approach to compare analytical data allows QC technicians to evaluate the seriousness of the detected error and make informed decisions about what action should be taken.

Results and Discussion

A Waters SQ Detector 2 with an Atmospheric Pressure Photo Ionization (APPI) source, coupled to an ACQUITY UPLC System, were used to acquire QC data for a blend of five polymer additives. The blend was comprised of: A. an antioxidant, Irganox 245; B. a UV absorber, 2-Hydroxy-4-(octyloxy)- benzophenone; C. a

plasticizer, Diethylhexyl phthalate (DEHP); D. a slip agent, Erucamide; and E. an optical brightener, Uvitex OB.



The SQ Detector 2 was operated in full scan mode to ensure that the acquisition was non-selective and that all of the ions formed were recorded. By using full scan mode, the analyst is able to ensure that any unexpected components are detected along with the expected compounds in the additive blend.

Figure 1 shows a QC sample matched to a master blend "Gold Standard". The Gold Standard represents the correct analytical profile of the polymer additive blend. The QC data can be overlaid on the Gold Standard data to see if the batch is of acceptable quality. In Figure 1, the QC spectrum clearly has one component peak missing and no unexpected peaks are observed. Here the blend only has four of the five required components – the UV absorber is missing. The QC technician can quickly identify that the batch is out of specification, and that the missing component is vital to the correct performance of the additive blend. In this case, the manufacturing run using this faulty batch can be stopped and corrective action can be taken.

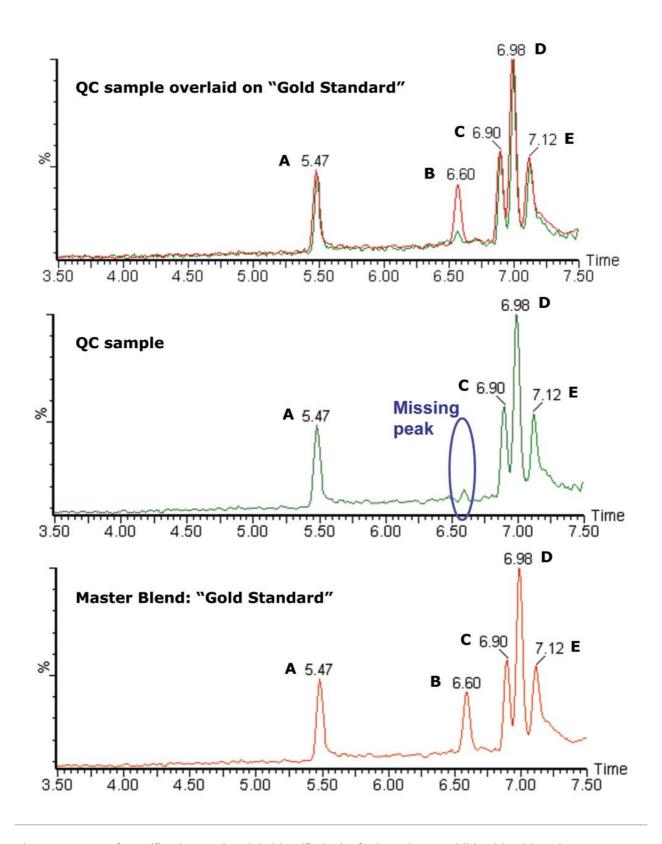


Figure 1. An out of specification QC batch is identified. The faulty polymer additive blend has the UV absorber 2-hydroxy-4-(octyloxy)-benzophenone missing and cannot be used in its current formulation.

Figure 2 shows an example in which the QC spectrum clearly has one component peak missing and one unexpected peak at a different retention time. The QC technician can interrogate the mass spectral data further and find the molecular mass of the unexpected component. The mass spectrum for the peak at 4.17 minutes shows an ion with m/z 226. This ion is characteristic of an alternative UV absorber, Tinuvin P. In this case, the error is benign and the additive blend can still be used.

Mass spectrum at 4.17 min 226.1 100-* 0 m/z 200 220 240 180 160 7.00 **QC** sample Unexpected 6.91 peak **Missing** peak % ז Time 3.50 4.00 6.50 6.00 7.00 4.50 5.00 5.50 7.50 6.99 Master Blend: "Gold Standard" 6.89 % 5.47 6.59 Time 4.00 4.50 7.00 5.00 5.50 6.00 6.50 3.50 7.50

Figure 2. A polymer additive blend has the UV absorber 2-hydroxy-4-(octyloxy)- benzophenone missing, but an alternative UV absorber, Tinuvin P, has been included instead. The batch can be used with this formulation.

Conclusion

The ACQUITY UPLC System, coupled to the SQ Detector 2 with an APPI source, were successfully used to acquire polymer additive QC data. Using the SQ Detector 2 in full scan mode enabled the acquisition of non-selective data and provided a complete picture of each QC sample.

Two different types of formulation error were quickly and easily detected, with little or no data processing required. An out of specification blend with a missing component was discovered and readily identified as unfit for purpose. A polymer additive blend with an unexpected component was also found. The unexpected component was identified as an acceptable substitute, so the batch could be used.

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SQ Detector 2 https://www.waters.com/134631584

ACQUITY UPLC System https://www.waters.com/514207

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