Intelligent System Emulation (ISET): New Possibilities in the Field of Method Development and Further Applications

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Introduction

Due to the introduction of UHPLC instruments to the market in the past few years the instrument-to-instrument method transferability has become an increasingly important topic.

Significant differences between UHPLC and HPLC systems can lead to notable changes in retention times and often in selectivity when methods developed on standard HPLC systems are run on modern UHPLC systems or vice versa.

As in many laboratories HPLC systems are slowly exchanged by UHPLC systems, an important requirement is the opportunity to transfer methods between labs of different divisions/locations, where various types of HPLC systems are used to develop methods as well as to carry out analytical measurements.

Method robustness testing

Testing a method for robustness against variation in instrument characteristics using just one instrument.

Method development

Develop methods for a variety of instruments on one 1290 Infinity instrument while maintaining individual instrument characteristics.

Perform existing methods

The range of instruments that can be emulated by ISET is continually extended in order to simplify the transfer of most of the existing methods to 1290 Infinity binary and quaternary systems. Figure 2 shows a method transfer from a Non-Agilent UHPLC system to a 1290 Infinity binary system by using ISET.

Robustness Test

An earlier approach to eliminate inter-laboratory transfer problems is robustness testing. It is used to indicate the capacity of an analytical method to be unaffected by small but deliberate variations in method parameters like pH and temperature.

Because of strict regulatory requirements it is mainly performed for pharmaceutical analyses and became an important part of method validation or method optimization.

Apart from test conditions such as temperature, different days or different analysts, the specific characteristics of various HPLC/UHPLC instruments have a high impact on method transferability. ISET offers the possibility to perform robustness testing also with respect to diversity of several HPLC instruments while using just one UHPLC instrument.

Figure 3 demonstrates a robustness test carried out with a 1290 Infinity System emulating four different HPLC instruments.

Method development

Another day-to-day use case is method development. ISET enables the user to establish a method for a variety of HPLC/UHPLC systems with just one instrument. Thus, it is not only possible to shorten the time frame but also to reduce the required instrument resources to a minimum.

Figure 4 depicts the performance of ISET utilized for the development of separation conditions of a pesticide sample. Emulated data include different types of instruments.

Conclusions

The transfer of analytical methodology between R&D contract research organizations and manufacturing as well as between different locations of one company is an essential part in the development of a new product.

ISET provides an easy-to-use solution for this requirement with regard to various use cases:

• perform existing methods
• develop new methods
• test a method for robustness