



PHYSICOCHEMICAL TESTING CASE STUDY

Handling Difficult Substances - Gases

Background

Gases, by their very nature, are difficult to handle and analyze. They are, however, generally bound by the same regulatory requirements as solid or liquid substances, so the same endpoint data is required. Physicochemical endpoints such as partition coefficient are requested because they are used to estimate the bioaccumulation potential of a substance. Yet the test guidelines for partition coefficient (OECD 107 and EC A8) are not designed with gases in mind, so procedures must be revised to enable adequate testing.

Our Physicochemical Testing Department was approached by a customer with a gas that was undergoing REACH registration. The customer needed a range of physicochemical endpoints assessed, including the partition coefficient.

The challenges

Established test guidelines (OECD 107 and EC A8) are primarily designed for solid and liquid substances and are unsuitable for gases, or even moderately volatile liquid substances. The main challenges faced in handling the gas related to the introduction of the gas to the test system and the prevention of losses from the system during introduction and analysis due to volatility.

The solution

Critical review of the test guidelines, coupled with extensive experience in partition coefficient testing, enabled us to establish where issues would arise and therefore what needed to be adjusted. The test guidelines recommend preparation of a stock solution of known concentration of test item in n-octanol, pre-saturated with water, which is then used to prepare the two-phase test systems at selected ratios. This approach is not generally practical for a gas and, therefore, instead of using a stock solution, each test system was individually dosed with gas at the appropriate concentration.

To prevent loss of the gas from the system, all sampling and handling was conducted in closed systems throughout. Initially, the gas was transferred to a gas-sampling bag. Samples were then removed via the septum of the bag using a gas-tight syringe and transferred to each two-phase test system, which were prepared in sealed headspace vials. Following mixing and centrifugation, samples of each phase were removed via the vial septum. After the n-octanol phase was sampled, the vial was carefully inverted and an aqueous phase sample removed. Both samples were immediately transferred to further sealed vials containing dilution or extraction solvent, as appropriate, to produce the final solutions for analysis.



Gases are generally:

- Difficult to handle
- Difficult to analyze
- Bound by the same requirements as solid or liquid substances

Conclusions

A pragmatic approach is required when considering how best to satisfy specific regulatory endpoints for a gaseous test substance. Some tests – such as surface tension – can justifiably be waived, but others, like partition coefficient, cannot. In the past, some regulatory endpoints may have been omitted simply because a substance is a gas, but greater regulatory scrutiny of missing data may mean these kinds of endpoints will become necessary for reapprovals. Where applicable, tests can be conducted successfully and regulatory requirements can be fulfilled by modification of the existing guidelines using a common-sense, science-led approach. In this particular case, a satisfactory mass balance was achieved using the modified procedure and the results were within the specification required by the test guideline.

Learn more at chemical.labcorp.com