

Transport Classification of Reactive Chemicals or how to balance Scientific Thinking against Business

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As an increasing number of chemicals is transported from one country to another, transport regulations gain more and more importance. Of special concern to us are the so called “self reacting chemicals”, which are classified as class 4.1 according to the “Recommendations on the Transport of Dangerous Goods” of the UN. A classification of a chemical in this class can result in a massive increase in transport costs and will even prohibit some methods of transport, e.g. airfreight.

To classify chemicals as “self reactive” essentially two measuring methods are proposed in the UN manual. Such methods should be scientifically sound and unambiguous, otherwise diverging results can be interpreted not in favour of transport safety but in favour of economics.

The first method is based on the assumption that a Dewar vessel of 200 ml is similar in heat loss to a transport package of 50 kg. Whether this is true depends on the quality of the experimental arrangement and on the physical properties and the physical state of the substance (liquid, solid, powdery). As both of these properties may vary, diverging results can be obtained.

The second method is based on the determination of the heat release kinetics of the decomposition using a set of different calorimetric measurements at a fixed temperature. Here self accelerating (“autocatalytic”) reactions make an application of this method difficult.

A case study explaining these difficulties is presented.

A complete study of the self reactivity of a chemical may be lengthy and the costs difficult to explain to the customer. Fast and comparatively simple screening methods are therefore needed.

A screening method for class 4.1 based on Differential Scanning Calorimetry for self reactivity is presented.

The early identification of self accelerating (“autocatalytic”) decomposition reactions is important. A screening method based on Differential Scanning Calorimetry showing whether a reaction might be autocatalytic or not was therefore developed and is presented.