

The Use of Impact Factors to Maintain Currency in an Evaluated Chemical Database

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A hallmark of the DIPPR[®] 801 pure chemical database is the extensive data evaluation performed to determine the best property values. The evaluation process is labor intensive and time consuming as it includes not only automated quality control checks, but also evaluation of experimental methods and techniques, analysis of inter-property consistency based on all known relationships, comparison of properties within chemical families, and consistent property trends with molecular structure. While this evaluation step is the foundation of the accuracy and consistency of property values in the DIPPR[®] 801 database, its labor-intensive nature makes maintaining currency of the recommended values problematic as new data continually become available. In this paper, we describe a system for efficiently determining the extent of re-evaluation warranted by newly published data. There are three components of the system: (1) data retrieval and entry of unevaluated data from current literature sources, (2) evaluation of the potential impact of the unevaluated data on the recommended values, and (3) rapid update of compound properties. Step 2 is key to the process. In the DIPPR[®] 801 implementation of this step discussed in this paper, a correlation for impact factors (IF) is used that includes weighting factors for the type of property, the experimental methodology, the quality of the data, the quantity of data upon which the current recommendation is based, and the significance of the potential change. An important side benefit of the deployment of this IF tool has been additional quality control on the database as a whole.