AMERICAN INSTITUTE OF CHEMICAL ENGINEERS
DESIGN INSTITUTE FOR PHYSICAL PROPERTIES

BYU - DIPPR®
Thermophysical Properties Laboratory
Department of Chemical Engineering
Brigham Young University
Provo, Utah 84602

P & P POLICIES AND PROCEDURES MANUAL

EVALUATED PROCESS DESIGN DATA

9 December 2011

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Evaluated Process Design Data Project

POLICIES AND PROCEDURES MANUAL FOR DIPPR PROJECT 801

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Introduction

The DIPPR (Design Institute for Physical Properties) 801 Project is an evaluated pure chemical database of the thermodynamic, physical, and transport properties (or thermophysical properties) for chemicals of high priority in industrial use. The objective of Project 801 is to provide a "Gold Standard" of thermophysical properties of unmatched quality and consistency for the most industrially important chemicals first to DIPPR sponsors and second to the general chemical process industry. The two defining characteristics of the DIPPR 801 database are:

1. Evaluation. While this term has been applied to other databases, its significance regarding the quality of data in the DIPPR 801 database is at a substantially higher level. All of the experimental property values obtained from the literature as well as predicted values are evaluated multiple times by thermodynamic experts at various levels of interdependence. At the narrowest level, individual values are evaluated in terms of quality based on chemical purity, experimental method, and potential errors. At a broader level, the property values are evaluated using known thermodynamic inter-relationships, rules of thumb obtained from experience, quality control algorithms, and the available DIPPR-approved prediction methods. At an even broader level, all properties are evaluated in terms of trends within chemical families and consistency with the values of related chemicals within the database. These levels of evaluation are repeated at least twice by two different groups: the Principal Investigators and their staff and by one or more of the industrial sponsors who often have experience with, interest in, or insights about the particular chemical or related chemicals. Review and approval of the recommended values and temperature-dependent correlations in the DIPPR 801 database by industrial sponsors is a unique and important distinction of the appellation "Evaluated Database." The same rigorous evaluation is used for predicted property values (see characteristic #2) as for experimental values.
2. Completeness. This term does not refer to the number of chemicals included in the database, but rather to the inclusion, whenever possible, of values for all of the constant properties and correlations for all of the temperature-dependent properties for every chemical included in the database. This requires that some properties which have not been measured are predicted by the Principal Investigators and their staff. The DIPPR philosophy is that engineers need thermophysical properties for design even if they have not or cannot be measured and the DIPPR 801 Principal Investigators are in the best position to make the most accurate recommendation of the property values based on their holistic analysis of all of the properties and their inter-relationships, their experience, and their continued evaluation of various prediction methods and their efficacy for specific types of chemicals.

This document presents the official procedural guidelines and methods approved by the DIPPR 801 sponsors and used by the project staff in dealing both with contents and format of this evaluated database. It serves as a guide for the staff to maintain consistency throughout the database and to apply consistent methods that have been tested and approved in the evaluation process. It is also intended to aid the project sponsors in supervising and steering the work of project 801. Additionally, advanced users of the database will find this manual a useful guide in understanding the database, how to use it efficiently, and the data analysis that has gone in to the database.

Revisions since June 2009 include:

- explanation of evaluation process (Section 4)
- explanation of Impact Factors (Section 6.3)
- explanation of Matrix Reviews (Section 6.5.3)
- update of policy on significant figures (Section 6.7)
- update of Quality Control Checks
- update of recommendations for critical property prediction methods
- update of recommendations for hazard property prediction methods
- update of recommendations for DC prediction methods
- update of HCOM conversion correlations

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