Technical Data Book: Chapter 2—Characterization of Hydrocarbons

API TECHNICAL REPORT TDB-2
FIRST EDITION, APRIL 2026



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Preface

This revised chapter is based on an expanded experimental database for petroleum characterizing parameters. Existing correlations were evaluated and new correlations for predicting some characterizing properties were developed. Correlations for aniline point, smoke point, freezing point, cloud point and cetane index were added to the chapter. Existing correlations for flash point, pour point and refractive index were evaluated and revised.

Scope

Technical Report TDB-2 provides methods for estimating characterization factors for pure components, petroleum fractions and mixtures that are common in refinery applications. Methods for estimating inspection properties of petroleum fractions are also included. Both computer algorithms and figures are presented for estimation of these properties. An estimate of the accuracy and range of application for most methods is presented.

Any references to other chapters within this document refer to the corresponding Technical Data Book Chapter which is published as API Technical Report TDB-x, where x is the chapter number.

2-0 Introduction

For correlational purposes, it is often necessary to designate the individual hydrocarbons in the various series by numerical parameters, which characterize them. The properties of methane, the smallest and the most spherical hydrocarbon, are well represented by the simple (two-parameter) corresponding states principle. But the molecules of larger hydrocarbons deviate from spherical symmetry, and thus we need to add to the corresponding states principle a third parameter as a measure of molecular size and shape. The most popular third parameter is the acentric factor (12, 13). The acentric factor is useful for correlating physical and thermodynamic properties and is defined as:

$$\omega = -\log p_r^* - 1.000 \qquad \textit{(2-0.1)}$$

Where:

p_r^*	=	*reduced vapor pressure, p*/p_c.*
p^*	=	*vapor pressure at T = 0.7 T_c, in psia.*
p_c	=	*critical pressure, in psia.*
T	=	*temperature, °R.*
T_c	=	*critical temperature, °R.*

The acentric factor is used in hydrocarbon correlations in several chapters of this book. Accordingly, Procedure 2A1.1 is presented as a general method of estimation consistent with Procedure 5A1.19. If experimental vapor pressure data are available, the defining equation (2-0.1) is recommended.

For mixtures of identifiable hydrocarbons, the acentric factor is given by the following equation:

$$\omega = \sum_{i=1}^{n} x_i \omega_i \qquad \textit{(2-0.2)}$$