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# Comparison of Corresponding-States-Based Correlations for the Prediction of the Vaporization Enthalpy of Fluids

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Four analytical correlations, including one proposed very recently, were used to calculate the enthalpy of vaporization of fluids. These correlations are based on the Pitzer et al. corresponding states principle and require as input the critical temperature and the acentric factor. They have generally been applied only to a reduced number of normal fluids (nonpolar, slightly polar, non-hydrogen-bonding, and nonquantum fluids), but in this paper we check their accuracy and applicability for 1594 polar and nonpolar fluids grouped into 81 families. The results are compared with the values accepted by the DIPPR project. Recommendations are given for the use of each model and for the choice of the adequate model for each family of fluids. In particular, we found that the most recent model, proposed by Morgan, gives the best results for most of the families and behaves better than the other models at both high and low temperatures.

## 1. Introduction

The enthalpy of vaporization of a pure fluid is a very important thermodynamic property that is required in processes involving a liquid–vapor change of phase such as distillation, evaporation, and drying, etc. Moreover, this property is sometimes used in the prediction or correlation of other thermodynamic properties. In the cases where experimental values are not known, empirical equations are used for their prediction. Indeed, there are many empirical correlations that allow one to calculate the enthalpy of vaporization of pure fluids.<sup>1–5</sup> Some of them include coefficients that must be calculated for each substance,<sup>6–10</sup> or the value of the enthalpy at a given temperature.<sup>11–15</sup> Others are general analytical expressions based on the corresponding states principle proposed by Pitzer et al.<sup>16</sup> and then only require as input parameters certain properties of the fluid, such as the critical temperature and the acentric factor,<sup>17–20</sup> or molecular parameters.<sup>21,22</sup> These correlations do not require the calculation of specific coefficients for each substance and thus can be regarded as predictive. The enthalpy of vaporization may also be predicted by means of group contribution models,<sup>23–27</sup> in which it is necessary to know the chemical groups in the molecule as well as its chemical structure.

In a recent paper<sup>28</sup> we made an overall comparison between the predictions given by four analytical models based on the corresponding states principle and the values accepted by the DIPPR project for 1576 substances.<sup>29–32</sup> Recommendations about the overall use of those models were given.

In another recent paper<sup>33</sup> Morgan has reviewed the correlations commonly used to fit properties in databanks (DIPPR in particular). As a result, a new corresponding-states-based model for the vaporization enthalpy has been proposed. The applicability and accuracy of this new model has not been studied for all the substances included in the DIPPR database. This model was not included in our previous analysis.<sup>28</sup>

In this work, we again check the applicability and accuracy of the corresponding-states-based models, but we have added results for 18 more substances and have grouped the substances

into 81 families. We then give more specific recommendations for the use of each model and for the choice of the appropriate model for each family of fluids. Moreover, the comparison performed illustrates the use of correlations to screen databases for potential problems.<sup>31,33</sup> In fact, we found several problems with respect to some of the data considered as accepted in the 2003 version of the DIPPR database,<sup>32</sup> some of which may perhaps have been corrected in the more recent versions.

The models used here are those proposed by Carruth and Kobayashi,<sup>17</sup> Sivaraman et al.,<sup>18</sup> Morgan and Kobayashi,<sup>19</sup> and Morgan.<sup>33</sup> All of them use the critical temperature and the acentric factor as inputs. The first three models have also been checked by us for the particular cases of the vaporization enthalpy at the standard and the boiling temperatures.<sup>34–36</sup> In the present work, those previous studies are completed by considering the whole temperature range.

In this paper the model proposed in refs 21 and 22, based on the use of molecular parameters, is not considered. In previous studies<sup>28,37</sup> we found that this model does not behave properly at either low or high temperatures. A more detailed analysis of the behavior of this model can be found in ref 37.

## 2. Correlations

We shall here only consider those analytical expressions that are based on the application of the corresponding-states principle<sup>16</sup> and that do not require specific adjustable coefficients for each substance or the value of the enthalpy at a given temperature, but rather knowledge of just two properties of each fluid: the critical temperature and the acentric factor. In particular, the acentric factor is used to interpolate and extrapolate dimensionless physical properties of some reference fluids.

The simplest of these expressions is that proposed by Carruth and Kobayashi,<sup>17</sup> which we shall call the “CK” correlation,

$$\frac{\Delta H_v}{RT_c} = 7.08(1 - T_r)^{0.354} + 10.95\omega(1 - T_r)^{0.456} \quad (1)$$

where  $T_r = T/T_c$  is a reduced temperature,  $T_c$  is the critical temperature,  $R$  is the universal gas constant, and  $\omega$  is the acentric factor.

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A more sophisticated model is that proposed by Sivaraman et al.,<sup>18</sup> which we shall call the “SMK” correlation. This model is based on Teja et al.’s<sup>38</sup> version of the corresponding-states principle and uses two fluids as reference: benzene, with  $\omega^{(R1)} = 0.21$ , and carbazol ( $C_{12}H_9N$ ), with  $\omega^{(R2)} = 0.46$ . The analytical expression of the SMK correlation is

$$\frac{\Delta H_v}{RT_c} = \left(\frac{\Delta H_v}{RT_c}\right)^{(R1)} + \left(\frac{\omega - \omega^{(R1)}}{\omega^{(R2)} - \omega^{(R1)}}\right) \left[\left(\frac{\Delta H_v}{RT_c}\right)^{(R2)} - \left(\frac{\Delta H_v}{RT_c}\right)^{(R1)}\right] \quad (2)$$

where  $(\Delta H_v/RT_c)^{(R1)}$  corresponds to the enthalpy of vaporization of benzene,

$$\begin{aligned} \left(\frac{\Delta H_v}{RT_c}\right)^{(R1)} = & 6.537(1 - T_r)^{1/3} - 2.467(1 - T_r)^{5/6} - \\ & 77.251(1 - T_r)^{1.208} + 59.534(1 - T_r) + \\ & 36.009(1 - T_r)^2 - 14.606(1 - T_r)^3 \end{aligned} \quad (3)$$

and the second term includes the difference between the benzene and carbazol enthalpies:

$$\begin{aligned} \left(\frac{\Delta H_v}{RT_c}\right)^{(R2)} - \left(\frac{\Delta H_v}{RT_c}\right)^{(R1)} = & -0.133(1 - T_r)^{1/3} - \\ & 28.215(1 - T_r)^{5/6} - 82.958(1 - T_r)^{1.208} + 99.000(1 - T_r) + \\ & 19.105(1 - T_r)^2 - 2.796(1 - T_r)^3 \end{aligned} \quad (4)$$

In principle, one would expect this correlation to perform especially well in predicting aromatic and heterocyclic aromatic ring structures, because of their similarity to the reference fluids. Nevertheless, no detailed analysis of families of fluids including substances with the aforementioned structures was performed.

Morgan and Kobayashi<sup>19</sup> used the three-parameter corresponding-states principle and proposed a model constructed by using data for alkanes and long-chain hydrocarbons. The correlation, which we shall call MK, is quadratic in the acentric factor:

$$\Delta H_v = \Delta H_v^{(0)} + \omega \Delta H_v^{(1)} + \omega^2 \Delta H_v^{(2)} \quad (5)$$

where each of the terms has the same analytical expression<sup>39</sup> as in eqs 3 and 4:

$$\begin{aligned} \frac{\Delta H_v^{(j)}}{RT_c} = & b_1^{(j)}(1 - T_r)^{1/3} + b_2^{(j)}(1 - T_r)^{5/6} + b_3^{(j)}(1 - T_r)^{1.2083} + \\ & b_4^{(j)}(1 - T_r) + b_5^{(j)}(1 - T_r)^2 + b_6^{(j)}(1 - T_r)^3 \end{aligned} \quad (6)$$

The 18 coefficients,  $b_i^{(j)}$  with  $j = 0, 1, 2$  and  $i = 1-6$ , were obtained by a fitting procedure and are listed by Morgan and Kobayashi.<sup>19</sup> They found average absolute deviations (AADs) of 2.2% compared to 10 (3 mmHg) boiling enthalpies of *n*-alkanes in the  $C_{21}$  to  $C_{43}$  range from Mazee<sup>40</sup> and 0.5% on the basis of extensive testing of 20 *n*-alkanes in the  $C_3$  to  $C_{28}$  range. Results of testing other compound classes were not presented.

Recently, Morgan<sup>33</sup> published a fit of the Pitzer et al.<sup>16</sup> tabular vaporization enthalpy correlation, which uses the same analytical form as is used in the DIPPR database:

$$\frac{\Delta H_v}{RT_c} = d_1(1 - T_r)^{d_2 + d_3 T_r + d_4 T_r^2} \quad (7)$$

where the coefficients  $d_i$  were fitted as cubic polynomial functions of the acentric factor:

$$\begin{aligned} d_1 = & 7.8149 + 11.409\omega + 2.1674\omega^2 - 0.65342\omega^3 \\ d_2 = & 0.81892 - 0.67637\omega + 1.2798\omega^2 - 0.47594\omega^3 \\ d_3 = & -0.84408 + 1.8297\omega - 3.2435\omega^2 + 1.1449\omega^3 \\ d_4 = & 0.41923 - 1.0892\omega + 1.9138\omega^2 - 0.65758\omega^3 \end{aligned} \quad (8)$$

In this fitting procedure, Morgan used 338 data in the ranges of  $0.56 \leq T_r \leq 1.0$  and  $0.0 \leq \omega \leq 1.2$ , obtaining AAD = 0.25%. The overall accuracy of the whole DIPPR accepted data set or for some particular fluids has not been studied.

In the present work, we studied the validity of these four models for the calculation of the enthalpy of vaporization. The predicted values are compared separately with those accepted in the DIPPR<sup>32</sup> database for 81 families of fluids. In principle, in the present comparison the M correlation has the advantage over previous models of using the same expression as is used in DIPPR. Nevertheless, the coefficients of eq 8 were obtained by using a reduced number of data and fluids, and therefore it is interesting to know whether those coefficients are adequate for other fluids and whether this new correlation clearly improves the results obtained with the previous models for all kind of fluids.

### 3. Results

Before making the comparison between the DIPPR accepted values and those predicted by the models, we carefully revised the DIPPR database. Thus, in our calculations we did not include those fluids for which there is no accepted value for the critical temperature, the value of the acentric factor is less than  $-1$ , or fewer than 5 accepted data are available in the DIPPR database. These last fluids (less than 5 data) were listed in ref 28.

Neither did we take into account the results obtained for another 21 fluids, most of them being acids or metals, for which very high AADs with respect to the accepted DIPPR data are found for each of the four predictive models used. Seventeen of these fluids are also listed in ref 28, and the other four are tri-*o*-cresyl phosphate, cuprous chloride, iron, and helium-3. This lack of agreement could be due to the need to use more specific correlations, or perhaps to unidentified mistakes in the DIPPR accepted data, the critical properties, or the acentric factor for those substances.

For another 88 fluids, we found that some of the accepted data do not agree with most of the rest of the data for the same fluid. These data were not considered in our comparison. The disagreement may be due to mistakes or because different sources give very different values; see ref 28. A list of data not considered is available upon request.

Finally, we carried out calculations for 1594 fluids, for which 47930 data were considered. The values of the critical temperature and acentric factor were taken from the DIPPR project.<sup>32</sup> The overall results are presented in Table 1, and separate results for 81 families of fluids (following the DIPPR nomenclature) are listed in Tables 2–7, where NF means number of fluids and ND means number of data for each family. We calculated the percentage deviation (PD) of the values obtained with each correlation model for each fluid at every temperature,  $\Delta H_i^m(T_i)$ , from those accepted by the DIPPR project,  $\Delta H_i$ , as follows:

$$PD_i = 100(\Delta H_i^m(T_i) - \Delta H_i)/\Delta H_i \quad (9)$$

Then we calculated the average absolute deviation (AAD) for each fluid  $j$ :

**Table 1. Overall Mean Absolute Percentage Deviations (OMAPD) for the 47930 Data Corresponding to 1594 Fluids, Percentage of Fluids with Negative Percentage Deviations (NPD) with Respect to the Values Provided by the DIPPR Database,<sup>32</sup> and the Percentage of Fluids for Which the Absolute Deviations (AADs, %) Are Less Than or Equal to a Given Value (CK = Carruth and Kobayashi,<sup>17</sup> Equation 1; SMK = Sivaraman et al.,<sup>18</sup> Equations 2–4; MK = Morgan and Kobayashi,<sup>19</sup> Equations 5 and 6; M = Morgan,<sup>33</sup> Equations 7 and 8)**

model	OMAPD (%)	NPD (%)	% of fluid for given AAD				
			≤1%	≤2.5%	≤5%	≤10%	>10%
CK	4.1	83.1	2.7	28.0	73.2	94.0	6.2
SMK	3.7	52.4	11.5	46.3	74.5	93.1	6.9
MK	3.6	37.5	14.8	53.8	77.7	92.0	8.0
M	3.3	45.4	27.2	57.9	78.4	92.1	7.9

**Table 2. Mean Absolute Percentage Deviations (MAPD) of the Values Obtained with the Models from the Values Provided by DIPPR<sup>32</sup> for Several Families of Fluids (NF = Number of Fluids; ND = Number of Data)<sup>a</sup>**

families	NF	ND	CK	SMK	MK	M
<i>n</i> -alkanes	32	1339	3.5	3.8	<b>2.0</b>	2.9
methylalkanes	17	613	2.6	1.6	<b>1.2</b>	<b>0.8</b>
dimethylalkanes	21	745	2.5	1.3	<b>0.9</b>	<b>0.7</b>
other alkanes	25	829	2.6	<b>1.5</b>	1.7	<b>1.0</b>
cycloalkanes	6	241	1.8	2.3	<b>1.1</b>	<b>1.1</b>
multiring cycloalkanes	3	83	<b>2.3</b>	<b>2.5</b>	<b>2.5</b>	<b>2.3</b>
alkylcyclopentanes	11	335	1.8	1.9	<b>1.5</b>	<b>1.2</b>
alkylcyclohexanes	16	510	4.4	<b>3.0</b>	<b>2.8</b>	<b>2.8</b>
1-alkenes	20	770	2.7	2.6	<b>1.5</b>	<b>1.6</b>
2,3,4-alkenes	24	696	3.0	2.0	<b>1.9</b>	<b>1.4</b>
methylalkenes	22	697	2.9	<b>2.0</b>	<b>1.7</b>	<b>1.5</b>
ethyl and higher alkenes	11	340	2.9	<b>2.1</b>	<b>1.8</b>	<b>1.7</b>
cycloalkenes	10	303	1.9	<b>1.7</b>	<b>1.8</b>	<b>1.3</b>
dialkenes	26	761	4.3	<b>3.9</b>	<b>3.9</b>	<b>3.6</b>
alkynes	18	550	<b>2.7</b>	3.1	<b>2.6</b>	<b>2.3</b>
<i>n</i> -alkylbenzenes	19	602	3.4	<b>2.2</b>	<b>2.2</b>	<b>1.8</b>
other alkylbenzenes	44	1496	3.1	<b>1.9</b>	<b>2.1</b>	<b>1.7</b>
other monoaromatics	16	521	3.2	<b>1.4</b>	<b>1.8</b>	<b>1.5</b>
naphthalenes	17	510	3.3	2.5	2.6	<b>1.7</b>
other condensed rings	10	284	4.6	3.8	<b>3.7</b>	<b>3.2</b>
diphenyl/polyaromatics	19	607	4.0	2.4	<b>1.7</b>	<b>1.4</b>
terpenes	6	189	2.9	<b>1.2</b>	1.9	<b>1.2</b>
other hydrocarbon rings	18	527	3.1	<b>2.3</b>	<b>2.0</b>	<b>1.9</b>

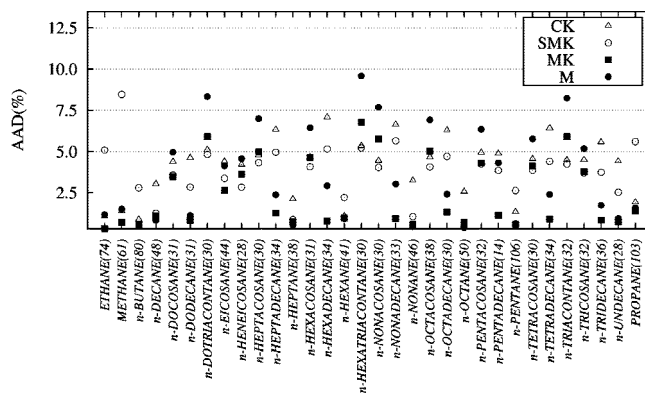
<sup>a</sup> Italic numbers represent the lowest MAPDs, and the numbers in bold are MAPDs that are similar (difference less than 0.5%) to the lowest one. CK= Carruth and Kobayashi,<sup>17</sup> eq 1; SMK= Sivaraman et al.,<sup>18</sup> eqs 2–4; MK = Morgan and Kobayashi,<sup>19</sup> eqs 5 and 6; M = Morgan,<sup>33</sup> eqs 7 and 8.

$$AAD_j = \frac{\sum_{i=1}^{ND_j} |PD_i|}{ND_j} \quad (10)$$

where  $ND_j$  is the number of available data for each fluid. Finally, we calculated the mean absolute percentage deviation (MAPD) for each family of fluids (i.e., by taking into account the number of available data for a family, ND, not the number of fluids for each family), and the overall MAPD (OMAPD), as follows:

$$MAPD = \frac{\sum_{i=1}^{ND} |PD_i|}{ND}, \quad OMAPD = \frac{\sum_{i=1}^{47930} |PD_i|}{47930} \quad (11)$$

In the analysis of the results, one must note that sometimes one finds two similar accepted values for the same or a very similar temperature. Moreover, for some fluids the number and the range of data available may be limited, whereas for other fluids one may find different data from different sources. Also, one has to bear in mind that when the temperature is close to



**Figure 1.** Absolute average percentage deviations (AAD, %) for the vaporization enthalpy of *n*-alkanes obtained using different correlations (see caption to Table 1). The number of available data for each fluid is given in parentheses.

the critical point, the vaporization enthalpy is near to zero, so that the percentage deviations of the models will be large even although the absolute deviations may generally be small.

Table 1 gives the overall MAPDs (OMAPD, in percent) for all the data considered, the percentage of fluids for which each model gives negative percentage deviations (NPD, in percent) with respect to the accepted DIPPR data,<sup>32</sup> and the distribution of the AADs, i.e., the percentage of fluids for which the AADs are less than a given value. As one can see, no model can reproduce all the accepted DIPPR data with AADs less than 10%. The simple CK model gives the highest OMAPD, overestimating the data for most of the fluids, and gives AADs ≤ 2.5% for only 28% of them.

The SMK and MK models give practically the same results. The SMK model gives NPDs for 52.4% of the fluids (this figure being 37.5% for the MK model). The distribution of AADs is also very similar. Finally, the M model gives the lowest OMAPD, although only with a minor improvement with respect to the others. The proportion of fluids with NPDs is near 50%, and this model can reproduce the data of 27.2% of fluids with AADs ≤ 1%, which is a considerable improvement when compared with the older models.

As the above results are not completely conclusive, it is worthwhile to test carefully the accuracy of each model for different families of fluids. The results and conclusions are given in the next subsections.

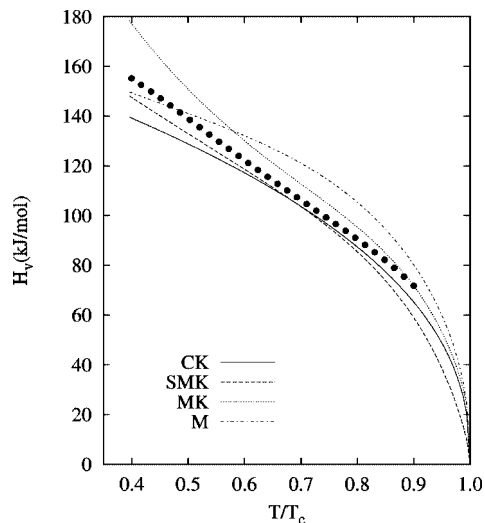
**3.1. Results for Alkanes, Alkenes, Aromatics, and Some Other Hydrocarbons.** As can be seen in Table 2, the MK model gives the lowest MAPD for *n*-alkanes. Figure 1 shows that AADs less than 7.5% are obtained for all the *n*-alkanes when this model is used. Nevertheless, there are 13 fluids for which the AADs obtained are greater than 2.5%. For these fluids the MK model predictions disagree with the data mainly at low temperatures, i.e., near the triple point. Moreover, for these fluids none of the models give low AADs either.

We note that the CK model also gives AADs below 7.5% for all the *n*-alkanes, but these deviations are below 2.5% only for seven fluids, so that a higher MAPD is obtained.

The recent M model gives good results for various fluids (see Figure 1), but it gives high AADs for several of them. Indeed, it does not give clearly better results than the MK model for any of the *n*-alkanes.

An extreme example of the poor behavior of the models for some of these fluids is shown in Figure 2. The curves in this figure are clear examples of how the analytical models behave when plotted versus the temperature. Although SMK and CK





**Figure 2.** Vaporization enthalpy for *n*-hexatriacontane versus the reduced temperature. Points are DIPPR data, and lines are values given using correlations.

give similar overall accuracy for this fluid (see Figure 1), in Figure 2 one can see that the CK model is further from the data than SMK at low temperatures but nearer at high temperatures. These different behaviors at low and high temperatures are clearly observed even for the simplest *n*-alkanes (ethane and methane), for which the SMK model gives inadequate results (see Figure 1).

In Figure 2 one also observes that the M model highly overpredicts the data at intermediate temperatures, because of an excessive curvature. This occurs for all the *n*-alkanes for which the M model gives medium or high AADs. Finally, one can see that the MK model predicts excessively high values at low temperatures, because it produces an inflection point at intermediate temperatures. This is a general behavior that can be observed in all the fluids for which there are data at low temperatures.

For methylalkanes, dimethylalkanes, and other alkanes, the CK model gives the highest deviation, whereas the use of the M model represents only a small overall improvement with respect to the SMK and MK ones. For most of the fluids, the MK model deviates clearly at the lowest temperatures, with the SMK and M ones giving better results.

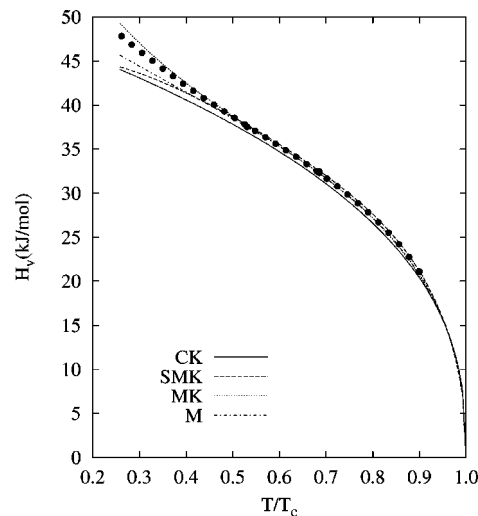
For some of these fluids the DIPPR data have an inflection point, with the vaporization enthalpy significantly increases at low temperatures. For these cases, the MK model is the only one capable of predicting that behavior. A clear example is shown in Figure 3.

Although SMK can reproduce the experimental data for cycloalkanes with AADs < 3.8%, they are the worst results for this family of fluids. Models MK and M give the best results, with AADs < 1.8% and PDs < 5.7%.

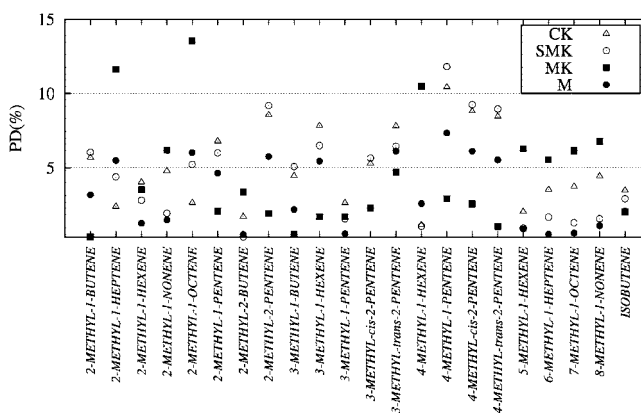
Only three multiring cycloalkanes have been considered, and the MAPDs found are very similar and always greater than 2.3%. The improvement of the most recent M model with respect to the older ones is almost inappreciable.

For alkylcyclopentanes the M model gives the best overall results, with a slight improvement over most of the others. The MK model should not be used for most of the fluids at low temperatures.

For alkylcyclohexanes the MAPDs obtained are clearly greater than those obtained for alkylcyclopentanes. The models must then be used with caution for the fluids of this family.



**Figure 3.** Vaporization enthalpy for 3,3-dimethylhexane versus the reduced temperature. Points are DIPPR data, and lines are values given using correlations.



**Figure 4.** Percentage deviations (PDs, %) for the vaporization enthalpy of methylalkenes at the lowest temperature obtained using different correlations.

Indeed, there are six fluids for which none of the models can adequately reproduce the data at intermediate and low temperatures. The greatest deviations are found for the two fluids listed in Appendix A.

The results for 1-alkenes and 2,3,4-alkenes using the different models are very similar, with the MK and M models giving the lowest MAPDs. In particular, the M model is the only one predicting the data for *trans*-2-eicosene and *trans*-2-pentadecene (AADs < 2% in both cases), with a clear improvement over the other models. It is worth noting that the SMK model gives poor results (AADs near 4%) for ethylene and propylene, with significant differences with respect to the other predictions. Finally, it must be taken into account that for some of these fluids (for instance, 1-octadecene, 1-tetradecene, 1-pentadecene, and especially 1-triacontene) very different results are obtained with each model.

For methylalkenes the M model slightly improves the overall results using SMK and MK, and it can reproduce all the data with PDs < 7.4%. These three models behave similarly at intermediate and high temperatures. Nevertheless, as can be seen in Figure 4, significant differences between them are found at low temperatures. The M model seems to be the only one giving PDs < 7.5% at the lowest temperature, and this leads to a lower MAPD. The MK gives the most heterogeneous results. There are eight fluids for which it gives poor results (PDs > 5%) at

the lowest temperatures, although there are nine other fluids for which it gives the lowest PDs.

For ethyl and higher alkenes the MK and M models give the best results, although their behaviors at low temperatures are different. We note that none of the models can adequately reproduce the available data for 2,3-dimethyl-2-butene.

For cycloalkenes the four models can be applied with good accuracy (AADs < 3%), with vinylcyclohexene being the only exception. As in the preceding families, the MK model must be used with caution at very low temperatures.

As can be seen in Table 2, none of the models give a low MAPD for dialkenes. All the models must be used with caution, because different results are obtained from one fluid to another. There are at least 10 dialkenes (see Appendix A) for which none of the models give low AADs, which is due mainly to clear disagreements at low temperatures. On the other hand, very good results are obtained for some other fluids of this family (examples are 1,4-hexadiene, methylcyclopentadiene, 1,5-hexadiene, and *trans,trans*-2,4-hexadiene).

For alkynes the four models give similar MAPDs, the lowest one being that given by the recent M model. Large deviations are found for 2-pentyne and 2-hexyne at low temperatures and for all the models. For three fluids, listed in Appendix A, major deviations are found for the whole temperature range.

As can be seen in Table 2, the M model slightly improves the overall results for *n*-alkylbenzenes obtained with the SMK and MK models. The improvement is significant for five fluids (*n*-hexadecylbenzene, *n*-pentadecylbenzene, *n*-heptadecylbenzene, *n*-octadecylbenzene, and *n*-tetradecylbenzene) for which the M model is the only one giving AADs below 2.9%.

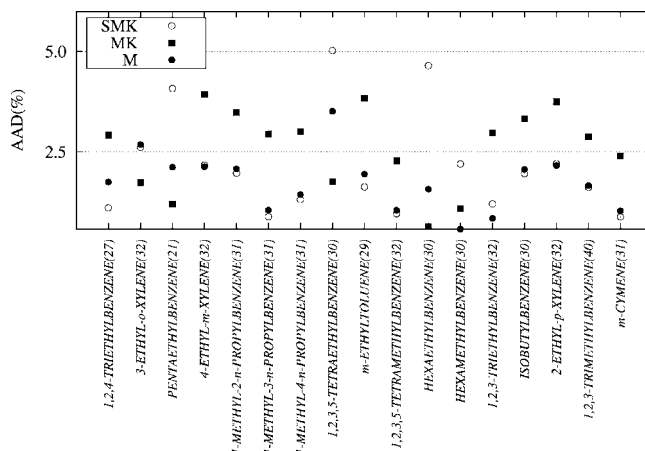
Special care must be taken with the use of the MK model, which does not reproduce adequately the data for seven fluids at the lowest temperature range. Moreover, we note that the data obtained from the SMK model do not agree with the accepted DIPPR values for benzene at reduced temperatures from 0.7 to 0.9. Because the SMK model was constructed using benzene as reference, eq 3, we must conclude that a different set of data or a different value for the critical temperature was used in that construction.

For other alkylbenzenes we found that, as is the case for most of the families, the new M model interpolates the behavior of the SMK and MK models at low temperatures (below reduced temperatures around 0.5) and thus gives a slightly lower MAPD. Figure 5 includes only those fluids for which a clear difference between the predictions given by the three aforementioned models is found. For these fluids, it is important to choose the model appropriately, due mainly to their different behaviors at low temperatures.

For other monoaromatics the SMK and M models give the lowest MAPDs. Nevertheless, the MK model is the only model that agrees with the DIPPR data for *o*-methylstyrene and *p*-methylstyrene at low temperatures.

Within the naphthalenes family, the worst results are obtained for naphthalene, for which none of the models can reproduce the DIPPR accepted data (AADs > 7.2%), especially at high temperatures. The M model gives the lowest MAPD, with a clear improvement over the other models for several fluids.

As can be seen in Table 2, for other condensed rings the SMK, MK, and M models give MAPDs around 3–4%, whereas the CK one gives 4.6%. It must be noted that no data are available at reduced temperatures below 0.4 and higher than 0.9, so that the behavior near the triple or the critical points cannot influence the results. In particular, for benzanthracene,



**Figure 5.** Absolute average percentage deviations (AAD, %) for the vaporization enthalpy of other alkylbenzenes obtained using different correlations. Only those fluids for which a clear difference between the predictions given by the three models is found have been included. The number of available data for each fluid is given in parentheses.

naphthalene, and chrysene, the M model clearly improves the results of the other models, giving AADs below 0.7%.

For diphenyl/polyaromatic substances each, a more recent model gives better overall results than the one that preceded it. Thus, the M model gives AADs ≤ 2.7%, except for *o*-terphenyl, for which all the models give AADs around 4–5%. In general, the MK model overpredicts the data for reduced temperatures below 0.5.

The best agreement with data for terpenes is found using the SMK and M models, which both lead to PDs < 3.5%. The MK model also gives good overall results, but it deviates clearly from the available data at low temperatures.

The M model gives slightly better overall results than the others for other hydrocarbon rings. The worst results are obtained for  $\alpha$ -pinene, for which none of the models reproduce the available data. Moreover, none of the models can reproduce the trend of the data (although low AADs are found with some of them) for 1-phenylindene and indene.

In sum, our results show that the four models selected reproduce the data for the 23 families of fluids included in Table 2 with MAPDs below 4.6%. The worst overall results are obtained for dialkenes, because different results are obtained from one fluid to another, and for other condensed rings, since the models cannot reproduce the data at intermediate temperatures. Moreover, we found that for several fluids, identified in the text and/or in the Appendix A, none of the models can reproduce the trend of the accepted DIPPR data over most of the temperature range, with there being particular disagreement at low temperatures.

Our results indicate that the M model gives the best overall results. A clear exception is the *n*-alkane family, for which the MK model clearly improves the results of the other models. In general, the degree of improvement of the M model with respect to the others is not significant, except for methylalkanes and naphthalenes.

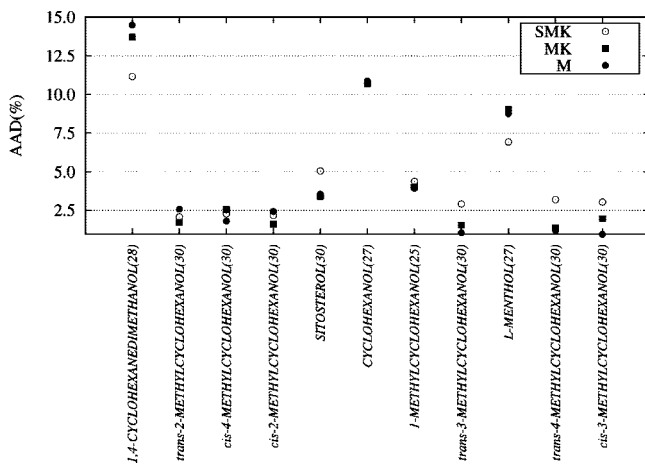
We also found that the MK model must be used with caution at low temperatures, because large deviations are found. Nevertheless, there are some fluids for which the DIPPR data have an inflection point, and then the vaporization enthalpy significantly increases at low temperatures. For most of these cases, the MK model is the only one capable of predicting that behavior.

**3.2. Results for Aldehydes, Ketones, and Alcohols.** Results for aldehydes, ketones, and five families of alcohols are

**Table 3. Mean Absolute Percentage Deviations (MAPD) of the Values Obtained with the Models from the Values Provided by DIPPR<sup>32</sup> for Several Families of Fluids (NF = Number of Fluids; ND = Number of Data)<sup>a</sup>**

families	NF	ND	CK	SMK	MK	M
aldehydes	32	942	3.2	<b>2.1</b>	<b>2.3</b>	<b>1.8</b>
ketones	35	1097	3.1	<b>1.9</b>	<b>2.2</b>	<b>1.9</b>
<i>n</i> -alcohols	20	558	10.6	9.1	<b>6.6</b>	7.9
cycloaliphatic alcohols	11	317	5.5	<b>4.8</b>	<b>4.5</b>	<b>4.5</b>
aromatic alcohols	33	925	<b>4.8</b>	<b>4.4</b>	<b>4.7</b>	6.2
other aliphatic alcohols	28	789	8.6	7.1	6.1	<b>4.5</b>
polyols	34	970	<b>7.0</b>	<b>7.2</b>	7.8	9.1

<sup>a</sup> See footnote <sup>a</sup> of Table 2 for explanation of bold and italic numbers and additional symbols.



**Figure 6.** Absolute average percentage deviations (AADs, %) for the vaporization enthalpy of cycloaliphatic alcohols obtained using different correlations. The number of available data for each fluid is given in parentheses.

presented in Table 3. As can be seen, for the first two families the SMK, MK, and M models give similar overall results (MAPDs around 2%), whereas CK gives the worst results.

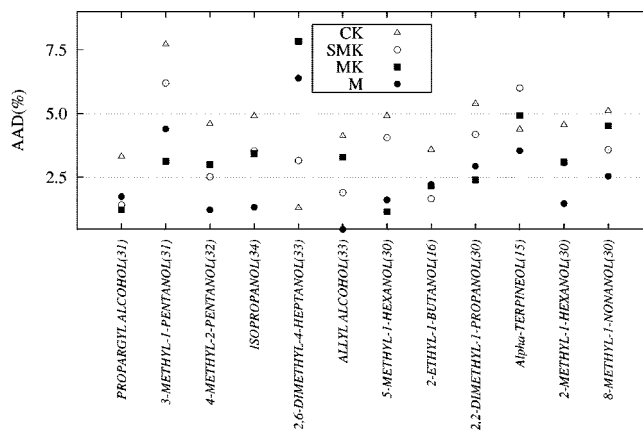
In the case of aldehydes, the M model clearly improves the agreement with DIPPR data when compared with the other models, for 2-ethylhexanal, 2-methylhexanal, terephthaldehyde, glutaraldehyde, and *p*-tolualdehyde. Despite the good results found for this family, none of the models accurately reproduce the trend of the data for five fluids, listed in Appendix A.

Similarly, none of the models agree with the DIPPR accepted data at low temperatures for the first five ketones listed in Appendix A, and over the whole temperature range for anthraquinone. Moreover, only the M model reproduces the data for 2,6,8-trimethyl-4-nonanone with a low AAD.

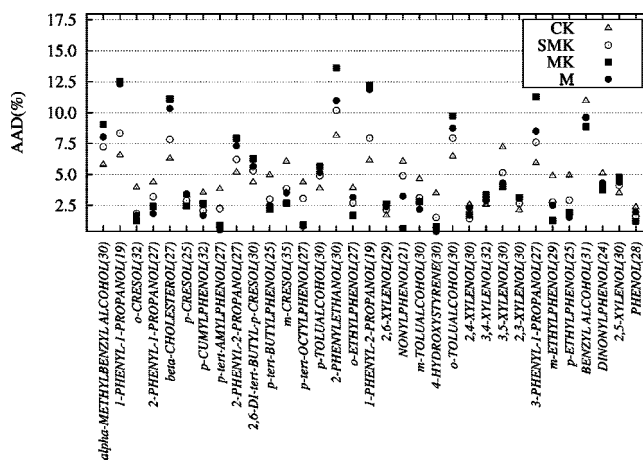
For the families of alcohols in Table 3, none of the models give MAPDs below 4.4%, with there being very large deviations for *n*-alcohols, other aliphatic alcohols, and polyols. As can be seen, for these families of alcohols the M model does not improve the predictions given by the oldest models. In particular, the MK model gives the best overall results for *n*-alcohols. Nevertheless, even with this model the AADs are always greater than 2%.

As can be seen in Figure 6, for cycloaliphatic alcohols the AADs obtained for each fluid take very different values, due to the different trend of the data. None of the models can reproduce the trend of the data for those fluids for which the data increase sharply at low temperatures or increase slowly at low temperatures. The names of those fluids are given in Figure 6, so they have not been included in Appendix A.

The situation described above is the same for other aliphatic alcohols. Only for those fluids included in Figure 7 can one



**Figure 7.** Absolute average percentage deviations (AADs, %) for the vaporization enthalpy of other aliphatic alcohols obtained using different correlations. Only fluids not included in Appendix A are shown. The number of available data for each fluid is given in parentheses.



**Figure 8.** Absolute average percentage deviations (AADs, %) for the vaporization enthalpy of aromatic alcohols. The number of available data for each fluid is given in parentheses.

find good agreement with the data (the others are listed in Appendix A). Moreover, we found that different choices of the appropriate model can lead to clearly different results for most of these fluids.

Large MAPDs were also obtained for aromatic alcohols and for polyols. In any case, for the first of these families there are several fluids for which good or even very good agreement with the accepted DIPPR data is found with all the models, as is shown in Figure 8 (phenol is a clear example). Nevertheless, the models do not agree for several others, which are listed in Figure 8, so they have not been included in Appendix A, with 2-phenylethanol and benzyl alcohol being the clearest examples.

The recent M model gives a clearly higher MAPD than the other models for polyols, with the CK model giving the best agreement. In any case, the CK model gives AADs  $\leq 3\%$  only for 1,3-propylene glycol, tripropylene glycol, and *p*-hydroquinone. Moreover, the CK model must be used with caution for some other fluids for which the most recent models give clearly lower AADs.

In sum, our results show that, despite the SMK, MK, and M models giving good overall results for aldehydes and ketones, these models should be used with caution for some particular fluids and/or some particular temperature ranges. For the five families of alcohols none of the models can be used with good overall accuracy, although good results can be obtained for some particular fluids, as described above.



**Table 4. Mean Absolute Percentage Deviations (MAPD) of the Values Obtained with the Models from the Values Provided by DIPPR<sup>32</sup> for Several Families of Fluids (NF = Number of Fluids; ND = Number of Data)<sup>a</sup>**

families	NF	ND	CK	SMK	MK	M
<i>n</i> -aliphatic acids	16	433	9.6	8.6	<b>4.6</b>	7.1
other aliphatic acids	21	566	5.8	4.8	<b>3.8</b>	<b>3.6</b>
dicarboxylic acids	14	413	5.5	5.8	<b>2.8</b>	4.5
aromatic carboxylic acids	10	293	6.2	6.6	<b>3.1</b>	6.1
anhydrides	9	263	<b>6.7</b>	7.8	9.7	8.8
formates	15	437	3.1	<b>2.3</b>	<b>2.6</b>	<b>2.2</b>
acetates	22	657	3.1	<b>2.0</b>	2.6	<b>1.9</b>
propionates and butyrates	13	384	3.4	<b>1.7</b>	<b>2.0</b>	<b>1.5</b>
other saturated aliphatic esters	21	520	<b>4.9</b>	<b>4.6</b>	5.7	<b>4.9</b>
unsaturated aliphatic esters	23	624	4.4	<b>3.5</b>	4.2	<b>3.3</b>
aromatic esters	29	813	4.8	<b>3.7</b>	4.4	<b>3.6</b>
aliphatic ethers	31	1021	2.1	<b>1.8</b>	2.2	<b>1.4</b>
other ethers/diethers	21	555	3.9	<b>3.2</b>	3.9	<b>3.2</b>

<sup>a</sup> See footnote *a* of Table 2 for explanation of bold and italic numbers and additional symbols.

**3.3. Results for Some Organic Acids, Anhydrides, Formates, Acetates, Propionates, Butyrates, Esters, and Ethers.** As can be seen in Table 4, none of the models can reproduce with accuracy the available data for *n*-aliphatic acids. The MK model gives the best overall results, but only for three acids of this kind (*n*-heptanoic acid, *n*-nonanoic acid, and *n*-octanoic acid) can this model reproduce the DIPPR data with AADs below 3%.

For other aliphatic acids, the MK and M models are the appropriate choice to reproduce the DIPPR data. In particular, for palustric acid, dehydroabiatic acid, and neoabiatic acid the MK model gives clearly lower AADs, whereas for 2-ethylbutyric acid, 2-methylbutyric acid, 2-methylhexanoic acid, and 2-methyloctanoic acid, the M model should be used, mainly because the MK model gives large deviations at low temperatures.

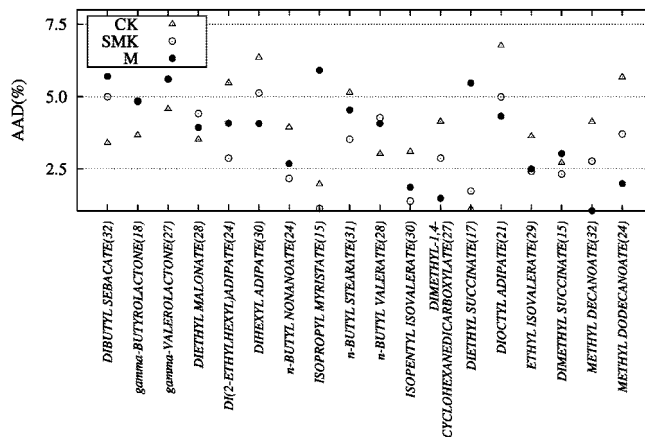
For both dicarboxylic acids and aromatic carboxylic acids the MK model clearly improves the overall results obtained with the other models. In any case, this model must be used with caution at low temperatures.

Table 4 shows that very poor agreement is found for anhydrides, no matter the model used. In particular, the CK model gives the lowest MAPD. Nevertheless, for three fluids only (butyric anhydride, propionic anhydride, and acetic anhydride) this model gives AADs  $\leq 4\%$ .

For formates, acetates, and propionates and butyrates the SMK, MK, and M models give similar results, the lowest values corresponding to the recent M model. In particular, we note that the CK model is the only one in agreement with the available data for *n*-pentyl formate and *n*-octyl acetate.

For the three families of esters included in Table 4, the SMK and M models give slightly better results than the others, but their MAPDs are always greater than 3.2%. In particular, the AADs obtained with the CK, SMK, and M models for the other saturated aliphatic esters not included in Appendix A are shown in Figure 9. As can be seen, the results are very inhomogeneous. Moreover, one can see that for most of the fluids the choice of one or another model leads to clearly different results. For those fluids for which these models give large deviations the MK model works similarly. We note also that for dioctyl adipate the MK model gives AAD = 2.3%, which is a clearly lower value than those shown in Figure 9.

Inhomogeneous results are also obtained for unsaturated aliphatic esters and aromatic esters. In particular, we found that for almost 50% of the fluids of these two families there is a clear disagreement between predictions and DIPPR data at low



**Figure 9.** Absolute average percentage deviations (AADs, %) for the vaporization enthalpy of other saturated aliphatic esters obtained using different correlations. Only fluids not included in Appendix A are shown. The number of available data for each fluid is given in parentheses.

temperatures or over the whole temperature range (for the latter case, the corresponding fluids are listed in Appendix A).

The four models give similar good overall accuracy for aliphatic ethers and not so good for other ethers and diethers. For aliphatic ethers the exception is di-*n*-pentyl ether, for which no model agrees with the DIPPR data at low temperatures.

Within the other ethers and diethers family, we found that the new M model clearly gives better results than the others only for triethylene glycol dimethyl ether and anethole. Apart from the exceptions listed in Appendix A, very good agreement is found for most of the fluids of this family.

In sum, we found a clear general disagreement between the data predicted by the models and the DIPPR accepted data for *n*-aliphatic acids, anhydrides, and other saturated aliphatic esters. For dicarboxylic acids and aromatic carboxylic acids the MK model clearly improves the results when compared with the other models. In any case, this model must be used with caution at low temperatures. Moreover, for 14 acids of these two families and of the other aliphatic acids family a clear disagreement is found whichever model is used.

For the other families we recommend the use of the SMK or M model because of their simplicity and slightly better results. In any case, the SMK model must be used with caution for esters, due to the results being very inhomogeneous (i.e., good or even very good agreement for some fluids and poor or even very poor agreement for others of the same family). It must also be used with caution at high temperatures.

**3.4. Results for Epoxides, Peroxides, Organic Chlorides, Amines, Imines, Nitriles, Isocyanates, and Diisocyanates; Mercaptans, Sulfides, and Thiophenes; and Nitroamines.** Results for 284 fluids grouped into 14 families are given in Table 5. Those fluids for which we have found clear overall disagreement between the predictions and most of the data are listed in Appendix A.

As can be seen, good results are obtained for epoxides with the four selected models, M (with AADs  $< 2.4\%$ ) slightly improving the results of the SMK and MK models. A clearer improvement is found for peroxides, for which the M model is the only one giving AADs  $< 2.8\%$ . Moreover, we observe that for most of the fluids the MK model does not agree with the DIPPR data at low temperatures.

For the three families of chlorides included in Table 5 the four models give MAPDs from 2.3 to 3.3%, the lowest values always corresponding to the M model. In particular, for 2-chloropropene and chloroprene the SMK model gives results



**Table 5. Mean Absolute Percentage Deviations (MAPD) of the Values Obtained with the Models from the Values Provided by DIPPR<sup>32</sup> for Several Families of Fluids (NF = Number of Fluids; ND = Number of Data)<sup>a</sup>**

families	NF	ND	CK	SMK	MK	M
epoxides	14	468	2.0	<b>1.7</b>	<b>1.4</b>	<b>1.3</b>
peroxides	11	302	4.6	3.1	2.6	<b>1.9</b>
C1/C2 aliphatic chlorides	19	674	<b>2.9</b>	3.1	<b>2.5</b>	<b>2.4</b>
C3 and higher aliphatic chlorides	26	725	3.3	<b>2.6</b>	<b>2.6</b>	<b>2.4</b>
aromatic chlorides	15	443	3.2	<b>2.4</b>	<b>2.4</b>	<b>2.3</b>
<i>n</i> -aliphatic primary amines	13	399	<b>3.3</b>	<b>3.2</b>	3.9	<b>3.6</b>
other aliphatic amines	20	475	4.4	<b>3.8</b>	4.1	<b>3.4</b>
aromatic amines	37	1119	3.4	<b>2.5</b>	<b>2.3</b>	<b>2.1</b>
other amines, imines	36	1081	4.3	<b>3.2</b>	<b>3.7</b>	<b>3.2</b>
nitriles	27	757	4.2	4.0	4.1	<b>3.2</b>
isocyanates/diisocyanates	10	275	4.5	<b>3.8</b>	4.8	<b>3.3</b>
mercaptans	23	691	2.3	1.7	<b>1.5</b>	<b>1.1</b>
sulfides/thiophenes	26	912	<b>2.4</b>	<b>2.0</b>	<b>2.2</b>	<b>1.9</b>
nitroamines	7	180	4.9	4.7	<b>4.0</b>	<b>4.4</b>

<sup>a</sup> See footnote *a* of Table 2 for explanation of bold and italic numbers and additional symbols.

in disagreement with the DIPPR data and with those obtained with the other models. Finally, we note that 25% of fluids of these kinds are included in Appendix A.

For *n*-aliphatic primary amines and other aliphatic amines we found that the SMK and M models give the lowest MAPDs, although with a slight difference with respect to the other models. In particular, for *n*-aliphatic primary amines the worst results are obtained for those fluids, listed in Appendix A, for which the four selected models overpredict the data at low temperatures and underpredict them at high temperatures. For *n*-octylamine two sets of data are accepted by DIPPR. Nevertheless we would note that the data tend to different critical points.

Within the other aliphatic amines family, the SMK model gives good results for di-2-ethylhexylamine, di-*n*-octylamine, diamylamine, triamylamine, and tri-*n*-butylamine at low temperatures but not at high temperatures, so that the M model should be used over the entire range.

The SMK, MK, and M models give similar overall accuracy for aromatic amines, with very good agreement for most of the 37 fluids of this kind. For other amines and imines, only for dehydroabietylamine, and triallylamine does the recent M model clearly improve the results of the other models. As in the previous families, the models must be used with caution at low and high temperatures for some fluids.

The M model gives the lowest MAPDs for nitriles, isocyanates, and diisocyanates; mercaptans; and sulfides and thiophenes. In particular, for nitriles the AADs obtained are below 4.1% except for the eight fluids included in Appendix A. For isocyanates and diisocyanates the use of the M model is recommended because of its good results over the whole temperature range for the five fluids not included in Appendix A: 1,5-naphthalene diisocyanate, *n*-butyl isocyanate, cyclohexyl isocyanate, isophorone diisocyanate, and methyl isocyanate. For mercaptans the M model can reproduce the data for the 23 fluids, with AADs less than 2.8%.

For sulfides and thiophenes the improvement obtained with the use of the M model is slight. In particular, for di-*n*-octyl sulfide the MK and M models give AADs greater than 5.5%, so that the CK or SMK models should be used. Moreover, for diethyl disulfide and di-*n*-propyl disulfide the CK model gives a significantly lower AAD than the other models. Finally, we note that for benzothiophene two different sets of data are accepted by DIPPR, but those data tend to different critical points.

**Table 6. Mean Absolute Percentage Deviations (MAPD) of the Values Obtained with the Models from the Values Provided by DIPPR<sup>32</sup> for Several Families of Fluids (NF = Number of Fluids; ND = Number of Data)<sup>a</sup>**

families	NF	ND	CK	SMK	MK	M
C, H, Br compounds	17	486	<b>4.6</b>	5.3	<b>5.0</b>	<b>4.6</b>
C, H, I compounds	8	248	<b>3.5</b>	5.1	4.8	4.3
C, H, F compounds	28	894	2.5	2.3	<b>1.7</b>	<b>1.6</b>
C, H, multihalogen compounds	37	1201	2.2	2.2	<b>1.4</b>	<b>1.3</b>
C, H, NO <sub>2</sub> compounds	21	510	<b>6.7</b>	8.3	10.7	10.4
polyfunctional acids	20	563	5.5	6.0	<b>3.9</b>	6.7
polyfunctional esters	23	617	<b>5.7</b>	<b>5.7</b>	8.0	7.5
other polyfunctional C, H, O	50	1341	<b>6.9</b>	<b>7.4</b>	9.3	8.6
polyfunctional nitriles	7	201	5.5	5.3	7.0	<b>4.7</b>
polyfunctional amides/amines	27	774	5.0	<b>4.1</b>	<b>3.8</b>	<b>4.1</b>
polyfunctional C, H, O, N	30	822	4.9	4.5	<b>3.5</b>	<b>3.6</b>
polyfunctional C, H, O, S	13	368	<b>4.1</b>	<b>3.7</b>	5.6	<b>4.1</b>
polyfunctional C, H, O, halide	34	947	4.1	<b>3.6</b>	4.0	<b>3.3</b>
polyfunctional C, H, N, halide, (O)	12	331	3.5	<b>2.8</b>	3.1	<b>2.3</b>
other polyfunctional organics	5	147	3.0	<b>1.5</b>	<b>1.9</b>	<b>1.6</b>

<sup>a</sup> See footnote *a* of Table 2 for explanation of bold and italic numbers and additional symbols.

**Table 7. Mean Absolute Percentage Deviations (MAPD) of the Values Obtained with the Models from the Values Provided by DIPPR<sup>32</sup> for Several Families of Fluids (NF = Number of Fluids; ND = Number of Data)<sup>a</sup>**

families	NF	ND	CK	SMK	MK	M
organic salts	16	456	<b>6.0</b>	7.2	8.8	7.8
silanes/siloxanes	37	1038	3.7	3.2	3.1	<b>2.5</b>
inorganic gases	23	748	<b>3.3</b>	<b>5.7</b>	<b>3.3</b>	<b>3.1</b>
inorganic halides	14	353	<b>6.8</b>	<b>7.2</b>	8.3	<b>7.3</b>
inorganic acids	4	139	<b>2.5</b>	5.9	3.1	<b>2.7</b>
inorganic bases (ammonia)	1	46	<b>1.6</b>	4.8	2.8	2.9
other inorganics	4	214	<b>2.3</b>	4.1	4.1	3.7
organic/inorganic compounds	6	151	6.2	<b>4.8</b>	5.7	<b>4.9</b>
elements	24	709	<b>6.3</b>	13.0	8.2	<b>6.4</b>

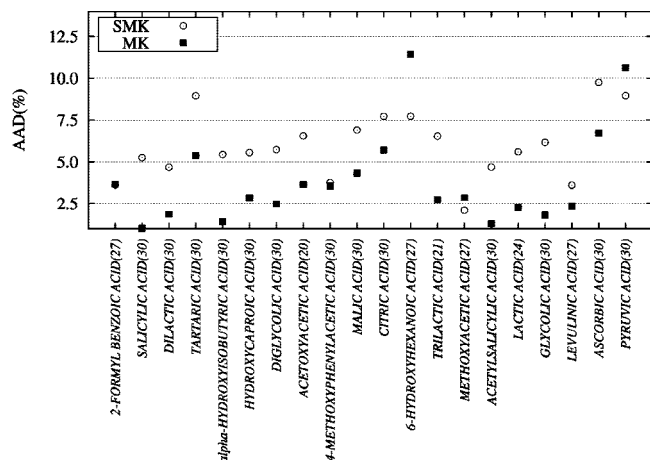
<sup>a</sup> See footnote *a* of Table 2 for explanation of bold and italic numbers and additional symbols.

No model gives a low MAPD when compared with the DIPPR data for nitroamines. In particular, for 4,4'-dinitrotriphenylamine, and 4,4'-dinitrodiphenylamine the MK model gives AADs clearly lower than those obtained with the other models. Two fluids of this kind are listed in Appendix A. For the remaining three fluids the models gives similar good agreement.

In sum, for the families of fluids listed in Table 5 we found similar MAPDs when the four models are used, with only minor exceptions. Only for some very specific fluids or families can the choice of one or another model represent a clear improvement in the agreement with the DIPPR data. In particular, for most of the fluids the use of the most recent M model means only a small improvement over the older models. In any case, we recommend the M model for overall use, due to its better behavior at extreme temperatures. We also found that there are a significant number of fluids of these families for which clear disagreement between the predictions of the models and the accepted DIPPR data is found over the whole temperature range. These fluids are included in Appendix A.

**3.5. Results for Other Compounds Containing Carbon and Hydrogen, and Other Polyfunctional Substances.** Table 6 summarizes the results obtained for other families of compounds containing carbon and hydrogen, and other polyfunctional substance families.

Large MAPDs are obtained for C—H—Br compounds, but it must be taken into account that the results are very inhomogeneous: the vaporization enthalpies of some fluids are accurately reproduced with most of the models, whereas clear disagreement is found for some other fluids.



**Figure 10.** Absolute average percentage deviations (AADs, %) for the vaporization enthalpy of polyfunctional acids obtained using different correlations. The number of available data for each fluid is given in parentheses.

For C–H–I compounds good agreement between predictions and data was found only for *n*-hexyl iodide and iodobenzene, with the CK and MK models, respectively, giving the lowest AADs.

Good agreement is found for C–H–F compounds, with the M and MK models giving slightly the best overall results. In particular, we found that the CK model is the only one giving an AAD < 1% for trifluoromethane and that the SMK model cannot reproduce the available data for 1,1-difluoroethylene.

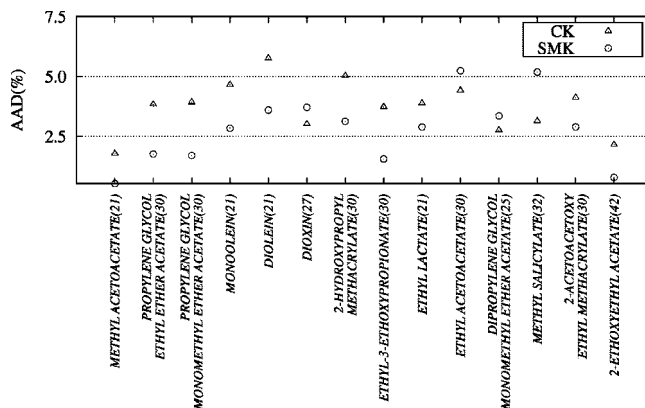
For 37 C–H–multihalogen compounds the MK and M models give the best overall results, although the former can give major deviations at low temperatures. Nevertheless, the SMK model is the only one that does not agree with the data for bromochlorodifluoromethane.

As can be seen in Table 6, none of the models can reproduce the DIPPR data for C–H–NO<sub>2</sub> compounds with an MAPD below 6.7%. In particular, for 2,4,6-trinitrotoluene, *o*-dinitrobenzene, *m*-dinitrobenzene, and *p*-dinitrobenzene the DIPPR accepted data do not go to zero near the critical point, so that not even the specific model proposed by DIPPR agrees with those data. Good agreement is found only for 1-nitrobutane when the CK model is used (AAD = 2%).

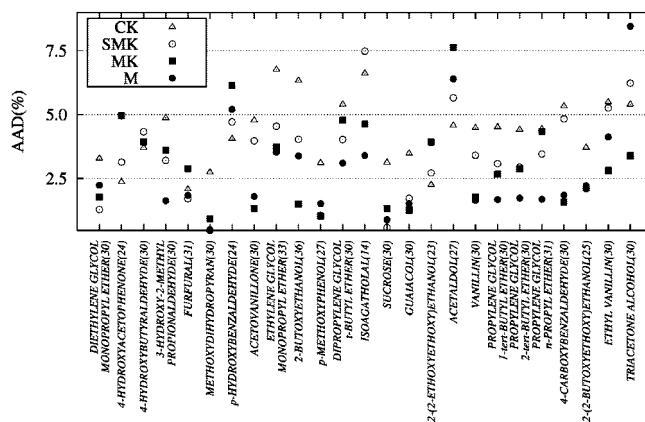
For polyfunctional acids we found that the recent M model gives the poorest overall results, whereas MK gives the best. As can be seen in Figure 10 even the MK model predictions clearly disagree with the data (AADs > 5%) for five fluids, which have been included in the Appendix. For some others, mainly those with AADs between 3 and 5%, the disagreement is found only at low temperatures. Finally, the MK model gives good or even very good agreement with data for the rest of the fluids, the improvement over the SMK results being clear.

Clear overall disagreement between predictions and data is found for polyfunctional esters, especially when the MK and M models are used. Nevertheless, these overall results are influenced by the very high AADs obtained for some particular fluids. For instance, the M model can reproduce the data of six fluids with AAD < 2%, but for diolein the AAD obtained is 27.9%.

Figure 11 shows the fluids of this kind for which the SMK model gives AADs below 6%. As can be seen, only for five of them are those AADs below 2.5%. In any case, Figure 11 shows that SMK must be the model selected for overall use, with methyl salicylate being the only notable exception.



**Figure 11.** Absolute average percentage deviations (AADs, %) for the vaporization enthalpy of polyfunctional esters obtained using different correlations. Only fluids for which the SMK model gives an AAD < 6% are included. The number of available data for each fluid is given in parentheses.

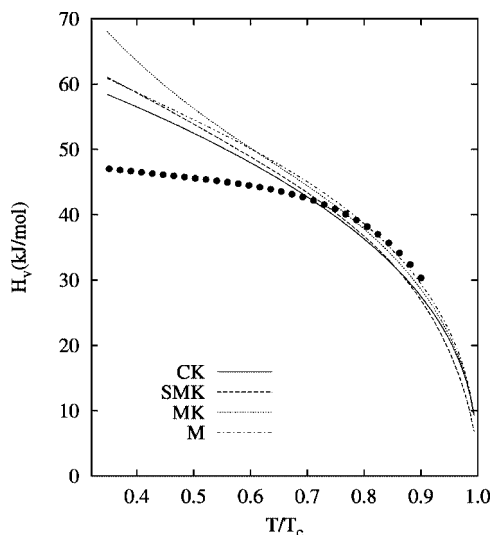


**Figure 12.** Absolute average percentage deviations (AADs, %) for the vaporization enthalpy of polyfunctional C–H–O substances obtained using different correlations. Only fluids not included in Appendix A are shown. The number of available data for each fluid is given in parentheses.

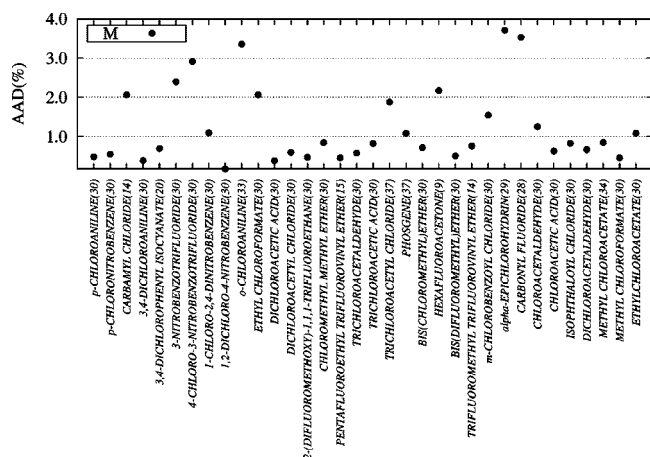
For other polyfunctional C–H–O substances we found that very different behaviors of dependence of the enthalpy on the temperature are given by the DIPPR project, so the models can only reproduce some of them. In particular, Figure 12 shows the AADs for the 25 out of 50 fluids of this kind for which there is at least one model giving an AAD less than 5% (the other 25 are listed in the Appendix). As can be seen, for some fluids there is a clear difference between the results given by each one of the models, so they must be selected carefully.

Despite the fact that for polyfunctional nitriles all the models give MAPDs greater than 4.6%, it must be taken into account that these overall results are clearly influenced by the extreme disagreement between the predicted values and the DIPPR data for hydracrylonitrile (AADs from 15.4 to 24.5%). For the other fluids, the AADs are below 5.2% except for the MK model, which gives the poorest overall results. This last model gives good results at high temperatures but not at low temperatures.

For polyfunctional amides/amines the MK model gives the best overall results, with only a minor difference with respect to the SMK and M models. Nevertheless, for *n,n*-diethylhydroxylamine, methylethanolamine, *tert*-butylformamide, and benzamide the M model gives the lowest AADs, with a clear difference with respect to the other models. Similarly, for 6-aminohexanol and 2-aminoethoxyethanol the MK model is clearly in better agreement with the data than the other models.



**Figure 13.** Vaporization enthalpy for 2-chloroethanol versus the reduced temperature. Points are DIPPR data, and lines are values given using correlations.



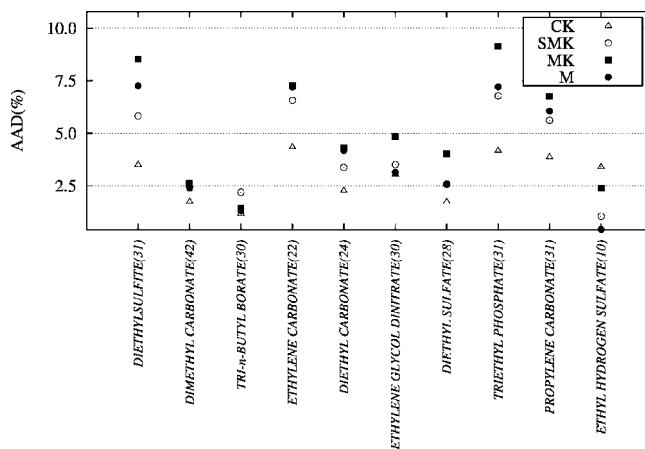
**Figure 14.** Absolute average percentage deviations (AADs, %) for the vaporization enthalpy of polyfunctional C–H–O–halide (the first ten fluids) and polyfunctional C–H–N–halide–(O) (the remaining ones) substances obtained using different correlations. Only fluids for which the M model gives AADs < 4% are shown. The number of available data for each fluid is given in parentheses.

For polyfunctional C–H–O–N substances the MK and M models give the lowest MAPDs. The improvement of MK over older models is clear in certain fluids. Nevertheless, it must be taken into account that this model does not agree with the data for some fluids at low temperatures.

For polyfunctional C–H–O–S fluids SMK gives the lowest MAPD, with the more recent models not improving its overall results. An exception is thiodiglycol, for which only the CK model gives good agreement with data.

For polyfunctional C–H–O–halide and polyfunctional C–H–N–halide–(O) substances the four models used give similar overall results, although the M model gives the lowest MAPDs. The greatest disagreement is found for those substances for which the DIPPR data values at low temperature are clearly lower than those predicted by the models. Figure 13 is a clear example. In Figure 14 we include the fluids of these two families for which AADs are lower than 4% when the M model is used. As can be seen, there are 20 fluids for which the agreement with data is excellent (AADs below 1%).

Finally, for other polyfunctional organic substances (only five substances were considered), we found that all the models give



**Figure 15.** Absolute average percentage deviations (AADs, %) for the vaporization enthalpy of organic salts obtained using different correlations. Only fluids for which there is at least one model giving AAD < 5% are shown. The number of available data for each fluid is given in parentheses.

good results. For this family, we recommend the use of the M model in order to avoid disagreement with the data at low temperatures.

In sum, we found a major overall disagreement (MAPDs greater than or equal to 3%) between the models and the data for most of the families of fluids included in Table 6. The CK model gives clearly lower MAPDs than the others for C–H–NO<sub>2</sub> compounds and less clearly for C–H–I compounds and other polyfunctional C–H–O substances. For polyfunctional acids only the MK model should be used. For the rest of the families, the M model gives similar or better results than the older models, and this should be the model used in order to ensure good overall predictions at both the lowest and the highest temperatures.

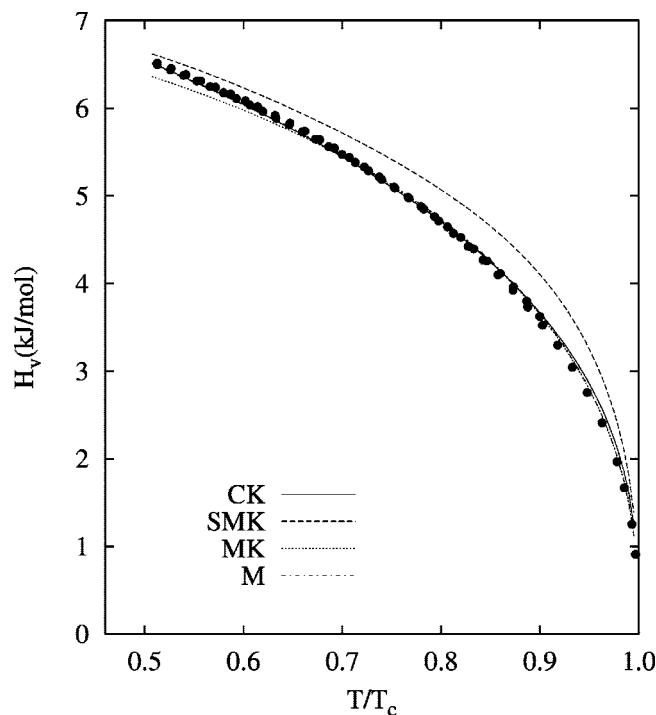
In any case, the results are very inhomogeneous within each family. Even for those families with a large MAPD, some models give good agreement with the data for certain fluids. The clearest disagreement is found for those fluids for which the DIPPR data do not go toward the accepted critical point or for which the enthalpy increases very quickly or very slowly when the temperature decreases.

**3.6. Results for Inorganic Compounds and Organic Salts.** Results for 129 inorganic compounds and organic salts, grouped into nine families, are summarized in Table 7. Those fluids for which a clear disagreement between the predictions and the trend of the data is found are listed in Appendix A.

For organic salts all the models give large MAPDs. In Figure 15 only the organic salts for which at least one of the models gives deviations below 5% are included. One observes that for most of these fluids the CK model gives the lowest AADs, due to the better overall behavior at different temperatures, with ethyl hydrogen sulfate being the only clear exception. The MK model does not behave properly at low temperatures and thus gives the greatest AADs.

For silanes and siloxanes the M model gives the lowest MAPD, this being slightly lower than the value obtained with the other models. Despite this good agreement, we found several fluids for which none of the models agree with the data at very low temperatures.

For inorganic gases we found that the SMK model gives the greatest MAPD, whereas the other models give similar overall results. This is due to the fact that the SMK model deviates clearly from the data and the other predicted values at



**Figure 16.** Vaporization enthalpy for carbon monoxide versus the reduced temperature. Points are DIPPR data, and lines are values given using correlations.

intermediate temperatures for several fluids. A clear example is shown in Figure 16. We also found that for hydrogen selenide, boron trichloride, and ozone no model agrees with the data at low temperatures, but good predictions are found at both intermediate and high temperatures.

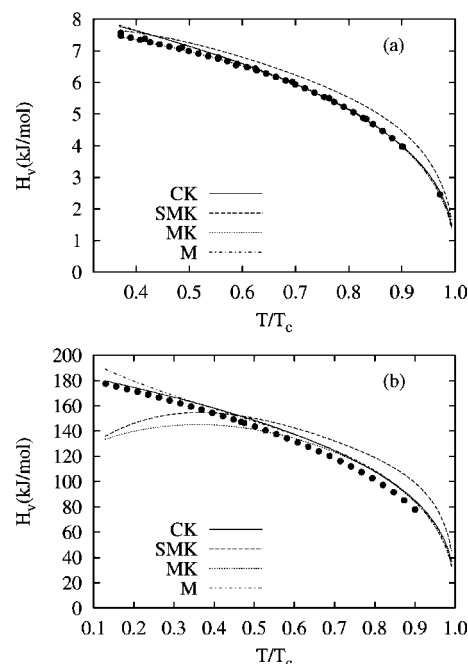
Very poor overall agreement between predicted values and data is found for inorganic halides (the complete list of inorganic halides has not been included in Appendix A). The dependence of the DIPPR data on the temperature varies drastically from one fluid to another, and the models only agree with the data over very limited temperature ranges and only for some particular substances.

For inorganic acids and the only inorganic base (ammonia) the CK model gives the lowest MAPDs, whereas SMK gives the greatest. Therefore the new models do not lead to better agreement.

Results for four other inorganic substances (hydrogen peroxide, deuterium oxide, arsenic trioxide, and water) were included in Table 7. The CK also gives the best agreement here, due to the fact that the predicted values at low temperatures are nearest to the data. None of the models agrees with the data for water at reduced temperatures below 0.6.

The SMK and M models give the lowest MAPD for some other organic/inorganic compounds. The agreement is good for four of them (triethyl aluminum, tetraethyl lead, methanesulfonyl chloride, and ethanesulfonyl chloride).

Finally, results for 24 simple elements are included in Table 7. As can be seen the SMK model gives clearly the greatest MAPD, whereas CK and M give the lowest. Clear examples of the behavior of these two models are shown in Figure 17. Figure 17a is also a clear example of the behavior of the SMK model. With respect to the MK model, it gives good results for several fluids even at low temperatures, as can be seen in the example of Figure 17a, but it deviates clearly from the data in those fluids for which there are data at very low temperatures (see Figure 17b). In particular, the MK model gives AADs of 1 and



**Figure 17.** Vaporization enthalpy for (a) fluorine and (b) lithium versus the reduced temperature. Points are DIPPR data, and lines are values given using correlations.

3.3% for *p*-hydrogen and hydrogen, respectively, whereas the others give AADs greater than 7.6 and 10.5%, respectively.

Clear disagreement is found between predictions and data for the nine fluids included in Appendix A. As Velasco et al.<sup>41</sup> have recently shown, new models with additional inputs are needed to achieve a good accuracy for some of these substances.

In sum, we found clear overall disagreement between the predictions given by all the models and the data for organic salts, inorganic halides, organic/inorganic compounds, and simple elements, with only a few exceptions for some particular fluids. The CK model should be used for inorganic bases and other inorganics (although these families included only four fluids in all), but can also be used for inorganic acids, inorganic gases, and simple elements.

For silanes and siloxanes, inorganic gases, inorganic acids, and simple elements the recent M model gives similar or better results than the other models, but moreover it has a better overall behavior over the whole temperature range. The MK model may be an alternative, although it must be used with caution at low temperatures. Finally, we have found that the SMK model seems to be clearly inadequate for overall use in the prediction of the vaporization enthalpy of most of the families included in Table 7, with the only exception of the silanes/siloxanes family. For some fluids the SMK model agrees with the data only at low temperatures, whereas MK does so only at high temperatures.

Finally, we note that for several fluids (most of them are listed in Appendix A) the DIPPR data are in clear disagreement with the values predicted by the models. The data for these fluids should be revised and confirmed, and then new models with additional inputs (similar to the proposal of Velasco et al.<sup>41</sup>) should be used to predict them.

## Conclusions

In the present work, we studied the validity of four models (CK, SMK, MK, and M) for the prediction of the enthalpy of vaporization. Results are compared with the values included in the DIPPR database for 1594 fluids grouped into 81 families.



Table 8. Fluids with Model Disagreement with DIPPR Data

other alkanes	other aliphatic alcohols	aliphatic ethers	nitriles	other polyfunctional C-H-O	polyfunctional C, H, O, halide (continued)
<b>alkylcyclohexanes</b> n-decylcyclohexane n-butylcyclohexane <b>1-alkenes</b> 1-triacetene <b>ethyl and higher alkenes</b> 2,3-dimethyl-2-butene <b>cycloalkenes</b> vinylcyclohexene <b>dialkenes</b> propadiene cyclopentadiene	<b>other aliphatic alcohols</b> 2-octanol 2-butanol 3-methyl-3-pentanol 2-pentanol 2-methyl-1-pentanol 2-hexanol 2-methyl-1-propanol 2-methyl-2-butanol 2-methyl-1-butanol 2-methyl-2-propanol 3-pentanol 3-methyl-1-butanol 2-ethyl-1-hexanol 2-heptanol 3-methyl-2-butanol 2-nonanol <b>other aliphatic acids</b> neopentanoic acid linoleic acid linolenic acid <i>cis</i> -crotonic acid oleic acid peracetic acid neopentanoic acid <b>dicarboxylic acids</b> sebacic acid azelaic acid suberic acid adipic acid <b>aromatic carboxylic acids</b> pyromellitic acid ibuprofen benzoic acid <b>formates</b> <i>n</i> -nonyl formate <i>n</i> -decyl formate <b>acetates</b> allyl acetate diethyl oxalate <b>other saturated aliphatic esters</b> $\epsilon$ -caprolactone $\beta$ -propiolactone <b>unsaturated aliphatic esters</b> 2-ethylhexyl acrylate ethylene glycol diacrylate methyl oleate isopropyl acrylate cetyl methacrylate diethyl maleate <b>aromatic esters</b> dimethyl isophthalate dimethyl terephthalate tri- <i>n</i> -heptyl trimellitate	<b>aliphatic ethers</b> di- <i>n</i> -pentyl ether <b>other ethers/diethers</b> acetal ethylal diethylene glycol di- <i>n</i> -butyl ether diphenyl ether tetraethylene glycol dimethyl ether <b>C1/C2 aliphatic chlorides</b> <i>cis</i> -1,2-dichloroethylene 1,1-dichloroethylene 1,1,2,2-tetrachloroethane vinyl chloride <b>C3 and higher aliphatic chlorides</b> 3,4-dichloro-1-butene hexachloro-1,3-butadiene 3-chloropropene 1,3-dichloro- <i>trans</i> -2-butene 2,3-dichloropropene <b>aromatic chlorides</b> 1,2,3-trichlorobenzene hexachlorobenzene <i>o</i> -dichlorobenzene benzyl chloride 1,3,5-trichlorobenzene 1-chloronaphthalene <b><i>n</i>-aliphatic primary amines</b> <i>n</i> -nonylamine <i>n</i> -dodecylamine <i>n</i> -tetradecylamine <i>n</i> -octylamine <i>n</i> -decylamine undecylamine <b>other aliphatic amines</b> diisobutylamine diisopropylamine tri- <i>n</i> -octylamine tripropylamine <b>aromatic amines</b> <i>n</i> -methylaniline <i>m</i> -phenylenediamine 2,6-diethylaniline phenylhydrazine <b>other amines, imines</b> diethylenetriamine tetraethylenepentamine hexamethylenediamine dicyclohexylamine pyridazine pyrimidine pentaethylene hexamine <i>n</i> -methylpyrrole ethyleneimine	<b>nitriles</b> glutaronitrile methacrylonitrile adiponitrile propionitrile hydrogen cyanide <i>trans</i> -crotonitrile acrylonitrile isocyanates/diisocyanates 2,4-toluene diisocyanate phenyl isocyanate 2,6-toluene diisocyanate 1,6-hexamethylene diisocyanate diphenylmethane-4,4'-diisocyanate <b>nitroamines</b> <i>p</i> -nitrophenylamine <i>p</i> -nitrodiphenylamine <b>C, H, Br compounds</b> 1-bromopropane bromoethane 1,1,2,2-tetrabromoethane vinyl bromide methyl bromide 1,1-dibromoethane <b>C, H, I compounds</b> diiodomethane <i>n</i> -propyl iodide ethyl iodide <i>n</i> -butyl iodide isopropyl iodide methyl iodide <b>C, H, F compounds</b> 3,3,3-trifluoropropene hexafluoropropylene <b>C, H, multihalogen compound</b> bromodifluoromethane <b>polyfunctional acids</b> tartaric acid citric acid 6-hydroxyhexanoic acid pyruvic acid <b>polyfunctional esters</b> 2-hydroxyethyl acrylate ethyl acetate methyl lactate 2-hydroxyethyl methacrylate ethylene glycol monobutyl ether acetate diethylene glycol ethyl ether acetate diethylene glycol monobutyl ether acetate 1,4-benzenedicarboxylic acid, bis(2,3-dihydroxypropyl) ester 2,2,4-trimethyl-1,3-pentanediol monoisobutyrate terephthalate	<b>other polyfunctional C-H-O</b> 2-methoxypropanol-1 2-(2-methoxyethoxy)ethanol 2-ethoxyethanol dextrose acetone alcohol tetrahydrofuryl alcohol ethylene glycol 2-ethylhexyl ether salicylaldehyde furfuryl alcohol 2,4-(2-butoxyethoxy)ethoxyethanol dipropylene glycol monoethyl ether dipropylene glycol monomethyl ether dipropylene glycol <i>n</i> -propyl ether 2-(2-ethoxyethoxy)ethoxyethanol 2,3-epoxy-1-propanol 2-(2-(2-methoxyethoxy)ethoxy)ethanol 1-isopropoxy-2-propanol tripropylene glycol monoethyl ether tripropylene glycol monomethyl ether 2-hexoxyethanol 2-hydroxyacetophenone propylene glycol monomethyl ether 2-(2-hexoxyethoxy)ethanol 2-methoxyethanol <b>polyfunctional nitrile</b> hydrazylonitrile <b>polyfunctional amides/amines</b> triethanolamine monoethanolamine <i>p</i> -dimethylaminobenzaldehyde diisopropylamine ethylenediaminetetraacetic acid 1-amino-2-propanol diethyl ethanolamine <b>polyfunctional C, H, O, N</b> acrolein cyanohydrin ethyl cyanoacetate succinimide nitroglycerine <b>polyfunctional C, H, O, S</b> thioglycolic acid ethylthioethanol 3-mercaptopropionic acid 2-mercaptoethanol <b>polyfunctional C, H, O, halide</b> 2,3-dichloro-1-propanol acetyl chloride 2-chloroethanol <i>m</i> -chlorophenol carbonyl fluoride bis(2-chloroethyl) ether	<b>polyfunctional C, H, O, halide (continued)</b> 3-chloro-1,2-propanediol <i>p</i> -chlorophenol $\alpha$ -epichlorohydrin benzoyl chloride 1,3-dichloro-2-propanol <b>polyfunctional C, H, N, halide, (O)</b> <i>o</i> -chloronitrobenzene <i>m</i> -chloronitrobenzene <b>organic salts</b> di- <i>n</i> -butyl sulfate trimethyl phosphate dimethyl sulfate ethylene carbonate dimethylaluminum chloride ethyl aluminum sesquichloride triphenyl phosphate <b>silanes/siloxanes</b> dimethyldimethoxysilane dichlorosilane dimethylchlorosilane silane methyl dichlorosilane diphenyldichlorosilane <b>inorganic gases</b> nitrosyl chloride tetrafluorohydrazine germanium tetrahydride chlorine dioxide organic/inorganic compounds trimethylgallium trimethylaluminum <b>elements</b> aluminum bismuth deuterium sodium potassium germanium mercury calcium beryllium

MAPDs for every family of fluids and every model were listed in separated tables for the convenience of the reader.

We have not considered various fluids and data of those included in the DIPPR database. The reasons are diverse (fewer than five available data, very large AADs, and clear disagreement between some of the data for the same fluid, etc.). Some of the nonconsidered fluids were already listed in ref 28. Finally, we note that for some fluids included in this work (most of which have been listed in Appendix A) the DIPPR data are in clear disagreement with the values predicted by all the models used here. The data for these fluids should be revised and confirmed, and then new models should be proposed.

An overall study of the data showed that the recent M model can slightly improve the results obtained with the previous models, being the only one giving AADs  $\leq 1\%$  for 27.2% of fluids. Nevertheless, this improvement does not extend to all kinds of fluids.

In general, the greatest disagreement between the predicted values and the DIPPR accepted data is found for those families for which the dependence of the vaporization enthalpy on the temperature is very inhomogeneous: it changes drastically from one fluid to another even although the fluids are of the same kind. In particular, major disagreement is found for those fluids for which the data at low temperatures increase either sharply or very slowly (with a very high or very low slope). Neither can the models predict the DIPPR accepted data which have a concave shape when plotted versus the temperature. Moreover, we found that all the models must be used with caution at low temperatures. Most of the fluids for which the greatest deviations are found have been clearly identified in the text, tables, and figures.

Although good results can be obtained for some particular fluids, none of the models can be used with good overall accuracy (MAPD  $\leq 3.0\%$ ) for dialkenes, other condensed rings, five families of alcohols, *n*-aliphatic and other aliphatic acids, aromatic carboxylic acids, anhydrides, three families of esters, other ethers and diethers, *n*-aliphatic primary amines, other aliphatic amines, other amines and imines, nitriles, isocyanates and diisocyanates, nitroamines, C–H–Br, C–H–I, and C–H–NO<sub>2</sub> compounds, and several polyfunctional families: acids, esters, nitriles, amides/amines, C–H–O, C–H–O–N, C–H–O–S, and C–H–O–halides. The same is the case for organic salts, inorganic halides, organic/inorganic compounds, and simple elements. Nevertheless, for some of these families the MAPDs obtained are in the range of 3–4% for at least one model.

Indeed, our results show that for 49 families at least three of the selected models reproduce the data with MAPDs below or equal to 4%. In any case, these models should be used with caution for some particular fluids and/or some particular temperature ranges. For these families the overall results are similar for the different models, with the degree of improvement of one model over another for the same family being not very high. There are, nevertheless, some exceptions within those 49 families. Thus, for instance, the SMK model gives a clearly greater MAPD than the other three models for inorganic gases, inorganic acids, inorganic bases (ammonia), and simple elements. The same is the case with the MK model for polyfunctional nitriles and polyfunctional C–H–O–S substances. In most cases, the disagreements are at low temperatures for both models.

For the other families (those not mentioned above) some models can give MAPDs of around 4–5%, and others can give higher values. Generally, this is due to the fact that the data for

fluids of the same family behave in different ways. The appropriate choice of one model is especially important for these families.

At was already shown in ref 28, the CK model gives the poorest overall accuracy. Nevertheless, we can now add that, despite this general result, the CK model gives clearly lower MAPDs than the others for anhydrides, C–H–NO<sub>2</sub> compounds, inorganic bases (ammonia), and other inorganics, and less clearly for organic salts. In any case, the results of the CK model are very inhomogeneous within each family.

With respect to the use of the MK and SMK models, we found that for some fluids the SMK model agrees with the data only at low temperatures, whereas MK does so only at high temperatures. Therefore the MK model must be used with caution at low temperatures (because for some fluids it predicts excessively high values) and the SMK model must be used with caution at high temperatures.

In a previous paper,<sup>28</sup> we recommended the use of the SMK model for overall reproduction of the DIPPR data. This conclusion was obtained by checking the model's overall accuracy for 1576 fluids and taking into account its simplicity. The new M model, however, was not considered.

Our results here indicate that, when separate families of fluids are considered, the SMK model gives good agreement for most families but does not clearly improve the overall agreement with the data when compared with the other models, for any of the families studied. However, the MK model is the only one giving a low MAPD for dicarboxylic acids and aromatic carboxylic acids and gives a clearly lower MAPD than the other models for *n*-alkanes, *n*-alcohols, and polyfunctional acids.

The recent M model gives the best agreement with the data for most of the families, although for all of them some other model can give similar results; i.e., there are no families for which this must be the only model to be used (as is the case of the CK and MK models for several families). Moreover, it is a simple model to use and its behavior at low and high temperatures is completely adequate, avoiding the poor behavior of the SMK and MK models in those ranges. Therefore, we must recommend the use of the M model except for those families cited above for which only the CK or the MK model give low MAPDs. Some other exceptions and particular uses have been mentioned in the different sections of this paper. Detailed tables and graphs for each fluid or family of fluids are available upon request.

Finally, we note that proposals of new models should focus on the prediction of the data for those families for which the simple corresponding-states-based models included here do not give sufficient accuracy.

## Acknowledgment

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## Appendix A

Fluids for which the prediction of the four models disagree with the DIPPR data are given in Table 8.

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