

# Reference Correlation of the Viscosity of *n*-Hexane from the Triple Point to 600 K and up to 100 MPa

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# Reference Correlation of the Viscosity of *n*-Hexane from the Triple Point to 600 K and up to 100 MPa

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This paper contains new, representative reference equations for the viscosity of *n*-hexane. The equations are based in part upon a body of experimental data that has been critically assessed for internal consistency and for agreement with theory whenever possible. The correlations are valid from the triple point to 600 K, and at pressures up to 100 MPa. We estimate the expanded uncertainty at a 95% confidence level to be 2% for the liquid phase at temperatures from the triple point to 450 K and pressures to 100 MPa. For the liquid at 450–600 K at pressures to 100 MPa, the expanded uncertainty at the 95% confidence level is 6%, and is 0.3% for the low-density gas at pressures to 0.3 MPa. © 2013 by the U.S. Secretary of Commerce on behalf of the United States. All rights reserved. [<http://dx.doi.org/10.1063/1.4818980>]

Key words: critical phenomena; *n*-hexane; transport properties; viscosity.

## CONTENTS

|                                                                          |    |
|--------------------------------------------------------------------------|----|
| 1. Introduction .....                                                    | 2  |
| 2. Methodology.....                                                      | 2  |
| 3. The Correlation.....                                                  | 2  |
| 3.1. The dilute-gas limit and the initial-density dependence terms ..... | 5  |
| 3.2. The critical enhancement term .....                                 | 6  |
| 3.3. The residual term.....                                              | 6  |
| 4. Computer-Program Verification.....                                    | 8  |
| 5. Conclusion .....                                                      | 10 |
| Acknowledgments .....                                                    | 10 |
| 6. References .....                                                      | 10 |

## List of Tables

|                                                                                       |   |
|---------------------------------------------------------------------------------------|---|
| 1. Viscosity measurements of <i>n</i> -hexane.....                                    | 3 |
| 2. Coefficients and parameters for Eqs. (3), (7), and (8) .....                       | 6 |
| 3. Evaluation of the <i>n</i> -hexane viscosity correlation for the primary data..... | 7 |

|                                                                                                     |    |
|-----------------------------------------------------------------------------------------------------|----|
| 4. Viscosity values of the liquid along the saturation line, calculated by the present scheme ..... | 9  |
| 5. Evaluation of the <i>n</i> -hexane viscosity correlation for the secondary data .....            | 9  |
| 6. Sample points for computer verification of the correlating equations .....                       | 10 |

## List of Figures

|                                                                                                                                                                                                                 |   |
|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---|
| 1. Temperature-pressure ranges of the primary experimental viscosity data for <i>n</i> -hexane.....                                                                                                             | 5 |
| 2. Temperature-density ranges of the primary experimental viscosity data for <i>n</i> -hexane.....                                                                                                              | 5 |
| 3. Comparison of the experimental values of $B_{\eta}$ for <i>n</i> -hexane with values calculated from Eqs. (2)–(7) with the parameters in Table 2. ....                                                       | 6 |
| 4. Percentage deviations of low-density viscosity ( $\Delta\eta_0 = \eta_0 + \eta_1 \rho$ ) experimental data of <i>n</i> -hexane from the values calculated by Eqs. (2)–(7) as a function of the density. .... | 6 |
| 5. Percentage deviations of primary experimental data of <i>n</i> -hexane from the values calculated by the present model as a function of density. ....                                                        | 7 |
| 6. Percentage deviations of primary experimental data of <i>n</i> -hexane from the values calculated by the present model as a function of temperature. ....                                                    | 7 |

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|     |                                                                                                                                                                |    |
|-----|----------------------------------------------------------------------------------------------------------------------------------------------------------------|----|
| 7.  | Percentage deviations of primary experimental data of <i>n</i> -hexane from the values calculated by the present model as a function of pressure.....          | 8  |
| 8.  | Percentage deviations of primary experimental data of <i>n</i> -hexane from the values calculated by the friction-theory model as a function of density. . .   | 8  |
| 9.  | Percentage deviations of primary experimental data of <i>n</i> -hexane from the values calculated by the friction-theory model as a function of temperature. . | 8  |
| 10. | Percentage deviations of primary experimental data of <i>n</i> -hexane from the values calculated by the friction-theory model as a function of pressure. .    | 8  |
| 11. | Viscosity of <i>n</i> -hexane as a function of temperature for selected pressures. ....                                                                        | 10 |

## 1. Introduction

In a series of recent papers, new reference correlations for the thermal conductivity of a series of fluids<sup>1–7</sup> covering a wide range of conditions of temperature and pressure were reported. In this paper, the methodology adopted for thermal conductivity is extended to developing a new reference correlation for the viscosity of *n*-hexane.

The goal of this work is to critically assess the available literature data, and provide a wide-ranging correlation for the viscosity of *n*-hexane that is valid over gas, liquid, and super-critical states, and that incorporates densities provided by a short-form equation of state (EOS) of Span and Wagner.<sup>8</sup>

## 2. Methodology

The viscosity  $\eta$  can be expressed<sup>9</sup> as the sum of four independent contributions, as

$$\eta(\rho, T) = \eta_0(T) + \eta_1(T)\rho + \Delta\eta(\rho, T) + \Delta\eta_c(\rho, T), \quad (1)$$

where  $\rho$  is the molar density,  $T$  is the absolute temperature, and the first term,  $\eta_0(T) = \eta(0, T)$ , is the contribution to the viscosity in the dilute-gas limit, where only two-body molecular interactions occur. The linear-in-density term,  $\eta_1(T)\rho$ , known as the initial density dependence term, can be separately established with the development of the Rainwater-Friend theory<sup>10–12</sup> for the transport properties of moderately dense gases. The critical enhancement term,  $\Delta\eta_c(\rho, T)$ , arises from the long-range density fluctuations that occur in a fluid near its critical point, which contribute to divergence of the viscosity at the critical point. Finally, the term  $\Delta\eta(\rho, T)$ , the residual term, represents the contribution of all other effects to the viscosity of the fluid at elevated densities including many-body collisions, molecular-velocity correlations, and collisional transfer.

The identification of these four separate contributions to the viscosity and to transport properties in general is useful because it is possible, to some extent, to treat  $\eta_0(T)$ ,  $\eta_1(T)$ , and  $\Delta\eta_c(\rho, T)$  theoretically. In addition, it is possible to derive information about both  $\eta_0(T)$  and  $\eta_1(T)$  from experiment. In contrast, there is little theoretical guidance concerning the

residual contribution,  $\Delta\eta(\rho, T)$ , and therefore its evaluation is based entirely on experimentally obtained data.

The analysis described above should be applied to the best available experimental data for the viscosity. Thus, a prerequisite to the analysis is a critical assessment of the experimental data. For this purpose, two categories of experimental data are defined: primary data, employed in the development of the correlation, and secondary data, used simply for comparison purposes. According to the recommendation adopted by the Subcommittee on Transport Properties (now known as The International Association for Transport Properties) of the International Union of Pure and Applied Chemistry, the primary data are identified by a well-established set of criteria.<sup>13</sup> These criteria have been successfully employed to establish standard reference values for the viscosity and thermal conductivity of fluids over wide ranges of conditions, with uncertainties in the range of 1%. However, in many cases, such a narrow definition unacceptably limits the range of the data representation. Consequently, within the primary data set, it is also necessary to include results that extend over a wide range of conditions, albeit with a poorer accuracy, provided they are consistent with other more accurate data or with theory. In all cases, the accuracy claimed for the final recommended data must reflect the estimated uncertainty in the primary information.

## 3. The Correlation

Table 1 summarizes, to the best of our knowledge, the experimental measurements<sup>14–20</sup> of the viscosity of *n*-hexane. We have included 107 sets in the table. From these sets, 10 were considered as primary data. Table 1 shows that most of the secondary data sets consist of a few measurements over a limited temperature range near ambient pressure and that many of the secondary data sets fail to provide the sample purity.

The data of Oliveira and Wakeham<sup>14</sup> and Assael *et al.*<sup>15</sup> were obtained in absolute vibrating-wire viscometers with an uncertainty of less than 0.5%, and these sets were considered as primary data. Also in the primary data set, the measurements of Berstad<sup>16</sup> and Knapstad *et al.*,<sup>17</sup> performed in absolute oscillating-cup instruments with 0.5% uncertainty at 0.1 MPa, rising to 1.1% at high pressures, were included. The measurements of *n*-hexane viscosity in the vapor phase of Vogel and Strehlow,<sup>19</sup> obtained in an absolute oscillating-disk viscometer with an uncertainty of 0.15%–0.30%, were also considered as primary data. Capillary viscometers were employed by Bauer and Meerlender<sup>20</sup> and Grigor'ev *et al.*,<sup>18</sup> with corresponding uncertainties 0.3% and 0.9%, and these two sets were also included in the primary data. Furthermore, the measurements of Dymond and Young<sup>21</sup> obtained in a capillary viscometer along the saturation line, with a 1% uncertainty, were also included in the primary data. Finally, after careful consideration, two more sets were included in order to extend the range of the correlation; the high-pressure measurements of Dymond *et al.*<sup>22</sup> obtained in a falling-body viscometer with a 2% uncertainty, and the measurements near the critical

TABLE 1. Viscosity measurements of *n*-hexane

| 1st author                  | Year of publication | Technique employed <sup>a</sup> | Purity (%) | Uncertainty (%) | No. of data | Temperature range (K) | Pressure range (MPa)  |
|-----------------------------|---------------------|---------------------------------|------------|-----------------|-------------|-----------------------|-----------------------|
| <b>Primary data</b>         |                     |                                 |            |                 |             |                       |                       |
| Oliveira <sup>14</sup>      | 1992                | VBW-Abs                         | 99.99      | 0.5             | 38          | 303–348               | 0.1–150 <sup>b</sup>  |
| Assael <sup>15</sup>        | 1991                | VBW-Abs                         | 99.00      | 0.5             | 15          | 298                   | 0.1–71                |
| Berstad <sup>16</sup>       | 1989                | OCup-Abs                        | 99.50      | 1.1             | 37          | 293–437               | 0.69–45               |
| Knapstad <sup>17</sup>      | 1989                | OCup-Abs                        | 99.00      | 0.5             | 7           | 288–327               | 0.1                   |
| Grigor'ev <sup>18</sup>     | 1988                | Cap                             | 99.29      | 0.9             | 53          | 178–323               | 0.1–59                |
| Vogel <sup>19</sup>         | 1988                | OD-Abs                          | 99.93      | 0.15–0.3        | 82          | 298–631               | 0.01–0.31             |
| Bauer <sup>20</sup>         | 1984                | Cap                             | 99.00      | 0.3             | 2           | 293–298               | 0.101                 |
| Dymond <sup>21</sup>        | 1980                | Cap                             | 99.00      | 1.0             | 12          | 283–393               | 0.01–0.4              |
| Dymond <sup>22</sup>        | 1980                | FB                              | 99.00      | 2.0             | 17          | 298–373               | 0.1–150 <sup>b</sup>  |
| Agaev <sup>23</sup>         | 1963                | Cap                             | 99.80      | 1–3             | 291         | 448–548 <sup>c</sup>  | 0.101–50 <sup>c</sup> |
| <b>Secondary data</b>       |                     |                                 |            |                 |             |                       |                       |
| Guerrero <sup>24</sup>      | 2011                | Cap                             | 99.00      | 2.0             | 4           | 283–313               | 0.101                 |
| Rathnam <sup>25</sup>       | 2010                | Cap                             | 99.00      | na              | 3           | 303–313               | 0.101                 |
| Dominguez <sup>26</sup>     | 2009                | Cap                             | 99.50      | na              | 1           | 298                   | 0.101                 |
| Feitosa <sup>27</sup>       | 2009                | VBT                             | 98.50      | 0.4             | 1           | 293                   | 0.101                 |
| Sastry <sup>28</sup>        | 2009                | Cap                             | na         | 0.3             | 2           | 298–308               | 0.101                 |
| Bandres <sup>29</sup>       | 2008                | Cap                             | 99.00      | 2.0             | 3           | 283–313               | 0.101                 |
| Fang <sup>30</sup>          | 2008                | Cap                             | 99.90      | 1.0             | 3           | 293–303               | 0.101                 |
| Shukla <sup>31</sup>        | 2008                | Cap                             | na         | 0.6             | 1           | 298                   | 0.101                 |
| Dubey <sup>32</sup>         | 2007                | Cap                             | 99.00      | 2.0             | 1           | 298                   | 0.10                  |
| Reddy <sup>33</sup>         | 2007                | Cap                             | 99.50      | 0.3             | 1           | 303                   | 0.101                 |
| Tian <sup>34</sup>          | 2007                | Cap                             | 99.40      | 1.0             | 8           | 293–328               | 0.101                 |
| Kumagai <sup>35</sup>       | 2006                | FB                              | 98.00      | 2.9             | 16          | 273–333               | 0.10–30               |
| Baragi <sup>36</sup>        | 2006                | VBT                             | 99.00      | 0.3             | 3           | 298–308               | 0.101                 |
| Iloukhani <sup>37</sup>     | 2006                | Cap                             | na         | 0.7             | 3           | 293–303               | 0.101                 |
| Modarress <sup>38</sup>     | 2006                | Cap                             | 99.00      | 0.3             | 3           | 298–313               | 0.101                 |
| Rodriguez <sup>39</sup>     | 2006                | Cap                             | 99.50      | 0.3             | 4           | 293–313               | 0.101                 |
| Al-Jimaz <sup>40</sup>      | 2005                | Cap                             | 99.00      | 1.0             | 3           | 293–303               | 0.10                  |
| Tripathi <sup>41</sup>      | 2005                | Cap                             | 99.00      | 1.0             | 1           | 298                   | 0.101                 |
| Yang <sup>42</sup>          | 2004                | Cap                             | 99.50      | 1.0             | 5           | 293–333               | 0.101                 |
| Bolotnikov <sup>43</sup>    | 2003                | Cap                             | 99.70      | 0.5             | 9           | 293–333               | 0.101                 |
| Dominguez <sup>44</sup>     | 2003                | Cap                             | 99.00      | 2.0             | 2           | 298–313               | 0.101                 |
| Nayak <sup>45</sup>         | 2003                | Cap                             | 99.00      | 0.3             | 3           | 298–308               | 0.101                 |
| Oswal <sup>46</sup>         | 2003                | Cap                             | 98.50      | 1.0             | 1           | 303                   | 0.10                  |
| Comelli <sup>47</sup>       | 2002                | Cap                             | 99.50      | 0.7             | 1           | 298                   | 0.101                 |
| Garcia <sup>48</sup>        | 2002                | RB                              | 99.50      | na              | 1           | 278–318               | 0.101                 |
| Peng <sup>49</sup>          | 2002                | Cap                             | 99.60      | 0.8             | 1           | 298                   | 0.101                 |
| Chowdhury <sup>50</sup>     | 2001                | Cap                             | 95.00      | 0.9             | 3           | 303–323               | 0.101                 |
| Gascon <sup>51</sup>        | 2001                | Cap                             | 99.00      | na              | 2           | 298–313               | 0.101                 |
| Postigo <sup>52</sup>       | 2001                | Cap                             | 99.50      | 1.7             | 3           | 283–313               | 0.101                 |
| Tu <sup>53</sup>            | 2001                | Cap                             | na         | 0.8             | 1           | 298                   | 0.101                 |
| Lal <sup>54</sup>           | 2000                | Cap                             | na         | na              | 1           | 298                   | 0.101                 |
| Aralaguppi <sup>55</sup>    | 1999                | Cap                             | 99.80      | 0.3             | 3           | 298–308               | 0.101                 |
| Barnes <sup>56</sup>        | 1999                | Cap                             | na         | 3.0             | 1           | 303                   | 0.101                 |
| Casas <sup>57</sup>         | 1998                | Cap                             | 99.00      | 0.1             | 1           | 298                   | 0.101                 |
| Aminabhavi <sup>58</sup>    | 1997                | Cap                             | 99.60      | 3.0             | 3           | 298–308               | 0.10                  |
| Nath <sup>59</sup>          | 1997                | na                              | na         | 0.7             | 1           | 298                   | 0.101                 |
| Orge <sup>60</sup>          | 1997                | FB                              | 99.00      | 2.0             | 1           | 298                   | 0.101                 |
| Sastry <sup>61</sup>        | 1996                | Cap                             | na         | 1.0             | 2           | 303–313               | 0.101                 |
| Aucejo <sup>62</sup>        | 1995                | Cap                             | 99.00      | 0.6             | 1           | 298                   | 0.10                  |
| Franjo <sup>63</sup>        | 1995                | Cap                             | 99.50      | 0.1             | 1           | 298                   | 0.101                 |
| Rived <sup>64</sup>         | 1995                | Cap                             | 99.00      | 0.1             | 1           | 303                   | 0.101                 |
| Papaioannou <sup>65</sup>   | 1994                | FB                              | 99.50      | 1.0             | 12          | 298                   | 0.10–52               |
| De Lorenzi <sup>66</sup>    | 1994                | Cap                             | 99.00      | na              | 1           | 298                   | 0.101                 |
| Kiran <sup>67</sup>         | 1992                | FB                              | 99.00      | 3.0             | 76          | 313–448               | 0.21–65.85            |
| Cooper <sup>68</sup>        | 1991                | Cap                             | na         | na              | 1           | 293                   | 0.101                 |
| Abdelraziq <sup>69</sup>    | 1990                | OQ                              | na         | 0.5             | 7           | 293–318               | 0.101                 |
| Chevalier <sup>70</sup>     | 1990                | Cap                             | na         | na              | 1           | 298                   | 0.101                 |
| Iwahashi <sup>71</sup>      | 1990                | Cap                             | 99.80      | na              | 2           | 298–323               | 0.101                 |
| Sekar <sup>72</sup>         | 1990                | Cap                             | na         | 0.5             | 1           | 303                   | 0.101                 |
| Grachev <sup>73</sup>       | 1989                | OCyl                            | 99.93      | 0.8–8           | 128         | 473–623               | 1–60                  |
| Schrodt <sup>74</sup>       | 1989                | Cap                             | na         | 0.2             | 1           | 297                   | 0.101                 |
| Chandrasekhar <sup>75</sup> | 1988                | Cap                             | na         | 1.0             | 1           | 303                   | 0.101                 |
| Rao <sup>76</sup>           | 1988                | Cap                             | na         | 0.5             | 1           | 298                   | 0.101                 |

TABLE 1. Viscosity measurements of *n*-hexane—Continued

| 1st author                 | Year of publication | Technique employed <sup>a</sup> | Purity (%) | Uncertainty (%) | No. of data | Temperature range (K) | Pressure range (MPa) |
|----------------------------|---------------------|---------------------------------|------------|-----------------|-------------|-----------------------|----------------------|
| Awad <sup>77</sup>         | 1986                | Cap                             | 99.50      | na              | 1           | 298                   | 0.101                |
| Craubner <sup>78</sup>     | 1986                | Cap                             | na         | na              | 1           | 293                   | 0.101                |
| Singh <sup>79</sup>        | 1985                | Cap                             | na         | na              | 1           | 298                   | 0.101                |
| Singh <sup>80</sup>        | 1984                | Cap                             | na         | 0.1             | 4           | 303–333               | 0.101                |
| Wei <sup>81</sup>          | 1984                | Cap                             | na         | na              | 1           | 298                   | 0.101                |
| Sreenivasulu <sup>82</sup> | 1982                | Cap                             | na         | 0.5             | 1           | 303                   | 0.101                |
| Kashiwagi <sup>83</sup>    | 1982                | TCr                             | 99.00      | 2.0             | 48          | 288–327               | 0.1                  |
| Asfour <sup>84</sup>       | 1981                | Cap                             | 99.00      | 1.7             | 1           | 298                   | 0.101                |
| Teja <sup>85</sup>         | 1981                | Cap                             | na         | 1.0             | 3           | 298–323               | 0.101                |
| Isdale <sup>86</sup>       | 1979                | FB                              | 99.00      | 2.0             | 29          | 298–373               | 0.1–500              |
| Gouel <sup>87</sup>        | 1978                | RB                              | na         | 5.0             | 51          | 292–393               | 0.1–40               |
| Medani <sup>88</sup>       | 1977                | RB                              | na         | na              | 12          | 353–463               | 0.14–1.53            |
| Bulanov <sup>89</sup>      | 1975                | Cap                             | na         | 1.0             | 60          | 373–473               | 0.11–2.53            |
| Diaz Pena <sup>90</sup>    | 1975                | Cap                             | 99.50      | na              | 9           | 323–408               | 0.05–0.55            |
| Moore <sup>91</sup>        | 1974                | Cap                             | na         | na              | 4           | 293–313               | 0.101                |
| Strumpf <sup>92</sup>      | 1974                | TCr                             | 99.00      | na              | 8           | 290–323               | 0.101                |
| Naziev <sup>93</sup>       | 1972                | Cap                             | na         | na              | 30          | 297–333               | 0.101–39             |
| Eicher <sup>94</sup>       | 1972                | Cap                             | 99.95      | 0.2             | 7           | 266–316               | 0.101                |
| Heric <sup>95</sup>        | 1972                | Cap                             | na         | 0.0             | 1           | 298                   | 0.101                |
| Ghai <sup>96</sup>         | 1971                | Cap                             | 99.95      | na              | 1           | 298                   | 0.101                |
| Ratcliff <sup>97</sup>     | 1971                | Cap                             | na         | na              | 1           | 298                   | 0.101                |
| Brazier <sup>98</sup>      | 1969                | FB                              | na         | na              | 3           | 273–333               | 0.1                  |
| Kuss <sup>99</sup>         | 1969                | Cap                             | 99.60      | 0.2             | 6           | 313                   | 0.1–148              |
| Johari <sup>100</sup>      | 1968                | Cap                             | na         | 1.0             | 1           | 298                   | 0.101                |
| Diaz Pena <sup>101</sup>   | 1967                | Cap                             | 99.50      | na              | 12          | 313–423               | 0.03–0.35            |
| Ridgway <sup>102</sup>     | 1967                | Cap                             | na         | 0.3             | 1           | 293                   | 0.101                |
| Parisot <sup>103</sup>     | 1961                | Cap                             | na         | 2.0             | 8           | 313–454               | 0.04–1.33            |
| Reed <sup>104</sup>        | 1959                | Cap                             | na         | na              | 1           | 298                   | 0.101                |
| Lambert <sup>105</sup>     | 1955                | Cap                             | na         | na              | 4           | 323–351               | 0.05–0.13            |
| Cummings <sup>106</sup>    | 1952                | Cap                             | na         | na              | 6           | 300–450               | 0.101                |
| Craven <sup>107</sup>      | 1951                | OPend                           | na         | 1.0             | 4           | 308–350               | 0.002                |
| McCoubrey <sup>108</sup>   | 1951                | Cap                             | na         | na              | 6           | 288–462               | 0.009                |
| Grunberg <sup>109</sup>    | 1950                | Na                              | na         | na              | 1           | 293                   | 0.101                |
| Giller <sup>110</sup>      | 1949                | Cap                             | na         | 0.5             | 14          | 174–293               | 0.101                |
| Geist <sup>111</sup>       | 1946                | Cap                             | na         | 0.1             | 3           | 273–313               | 0.101                |
| Khalilov <sup>112</sup>    | 1939                | Cap                             | na         | na              | 15          | 323–463               | 0.05–1.54            |
| Andrade <sup>113</sup>     | 1936                | OSph                            | na         | na              | 2           | 273–295               | 0.10                 |
| Titani <sup>114</sup>      | 1933                | Cap                             | na         | na              | 7           | 393–579               | 0.406–2.5            |
| Shepard <sup>115</sup>     | 1931                | Cap                             | na         | 0.5             | 1           | 298                   | 0.101                |
| Timmermans <sup>116</sup>  | 1928                | na                              | na         | na              | 2           | 288, 303              | 0.101                |
| Bridgman <sup>117</sup>    | 1926                | FB                              | na         | 10.0            | 1           | 303                   | 0.101                |
| Batschinski <sup>118</sup> | 1913                | Cap                             | na         | na              | 7           | 273–333               | 0.101                |
| Drapier <sup>119</sup>     | 1911                | Cap                             | na         | na              | 5           | 289–296               | 0.01–0.02            |
| Thorpe <sup>120</sup>      | 1894                | Cap                             | na         | na              | 7           | 273–333               | 0.101                |

<sup>a</sup>Abs, Absolute; Cap, Capillary; FB, Falling Body; na, not available; OCup, Oscillating Cup; OCyl, Oscillating Cylinder; OD, Oscillating Disk; OQ, Oscillating Quartz; OPend, Oscillating Pendulum; OSph, Oscillating Sphere; RB, Rolling Ball; TCr, Torsional Crystal; VBT, Vibrating Tube; VBW, Vibrating Wire.

<sup>b</sup>Data restricted to 150 MPa.

<sup>c</sup>Data within 0.2 K of the critical temperature and within 0.1 MPa of the critical pressure were excluded.

temperature of Agaev and Golubev<sup>23</sup> obtained in a capillary viscometer with an uncertainty of 1%–3%.

Figures 1 and 2 show the ranges of the primary measurements outlined in Table 1. The phase of the data, as well as the lack of measurements around the critical point, are apparent. Temperatures for all data were converted to the ITS-90 temperature scale.<sup>121</sup> The development of the correlation requires densities; Span and Wagner<sup>8</sup> in 2003 reviewed the thermodynamic properties of *n*-hexane and developed an accurate, wide-ranging equation of state up to 600 K and

100 MPa, with an uncertainty of 0.2% to 0.5% in density. Dymond *et al.*<sup>122</sup> measured the density of *n*-hexane from 298 to 373 K and up to 500 MPa, with an uncertainty of better than 0.04% at high pressures. To test the pressure extrapolation behavior of the equation of Span and Wagner<sup>8</sup> up to 500 MPa, we compared the densities computed from the EOS with the density measurements of Dymond *et al.*,<sup>122</sup> and found that although the EOS behaves in a physically reasonable manner to 500 MPa and 1000 K, the experimental liquid-phase densities of Dymond *et al.*<sup>122</sup> differ from those calculated from the



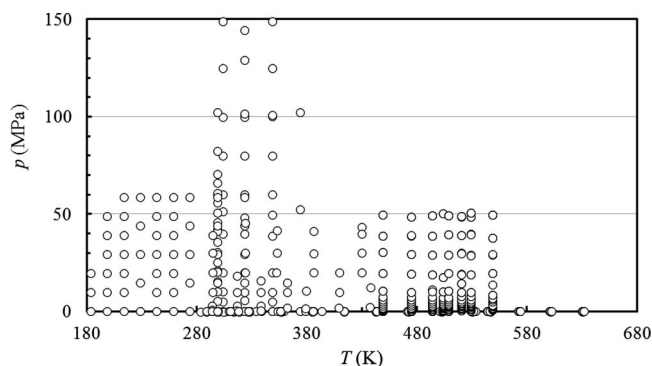


Fig. 1. Temperature-pressure ranges of the primary experimental viscosity data for *n*-hexane.

equation of state by as much as 1% at 500 MPa. This can be acceptable for thermal conductivity correlations,<sup>5</sup> but for the viscosity it can result in a much larger error. Hence, the equation of Span and Wagner<sup>8</sup> was employed up to its original limits, that is, 600 K and 100 MPa—limits that also restrict the present viscosity correlation. In addition, deviations for the density in the critical region are much higher. We also adopt the values for the critical point and triple point from their EOS; the critical temperature,  $T_c$ , and the critical density,  $\rho_c$ , were taken to be equal to 507.82 K and 233.182 kg m<sup>-3</sup>, respectively. The triple-point temperature is 177.83 K, and the molar mass is 86.17536 g mol<sup>-1</sup>.<sup>8</sup>

### 3.1. The dilute-gas limit and the initial-density dependence terms

The dilute-gas limit viscosity,  $\eta_0(T)$  in  $\mu\text{Pa s}$ , can be analyzed independently of all other contributions in Eq. (1). According to the kinetic theory, the viscosity of a pure polyatomic gas may be related to an effective collision cross section, which contains all the dynamic and statistical information about the binary collision. For practical purposes, this relation is formally identical to that of monatomic gases and can be written as<sup>123</sup>

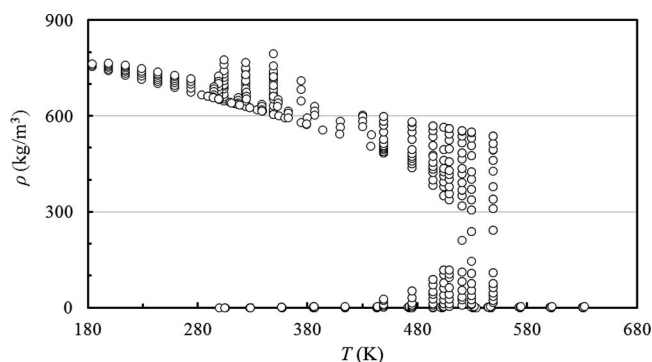


Fig. 2. Temperature-density ranges of the primary experimental viscosity data for *n*-hexane.

$$\eta_0(T) = \frac{0.021357\sqrt{MT}}{\sigma^2 S_\eta^*(T^*)}, \quad (2)$$

where  $S_\eta^* = S(2000)/(\pi\sigma^2 f_\eta)$  is a reduced effective cross section,  $M$  is the molar mass in g mol<sup>-1</sup>,  $\sigma$  is the length scaling parameter in nm, and  $f_\eta$  is a dimensionless higher-order correction factor according to Chapman and Cowling.<sup>124</sup> In the above equation,  $S(2000)$  is a generalized cross section that includes all of the information about the dynamics of the binary collisions that govern transport properties, which in turn are governed by the intermolecular potential-energy surface.<sup>123</sup> The effective cross section is usually expressed in the functional form

$$\ln S_\eta^*(T^*) = \sum_i \alpha_i (\ln T^*)^i, \quad (3)$$

$$T^* = k_B T / \varepsilon, \quad (4)$$

where  $T^*$  is the reduced temperature,  $\varepsilon/k_B$  is an energy scaling parameter in K, and  $k_B$  is Boltzmann's constant.

The temperature dependence of the linear-in-density coefficient of the viscosity,  $\eta_1(T)$  in Eq. (1), is very large at subcritical temperatures and must be taken into account to obtain an accurate representation of the behavior of the viscosity in the vapor phase. It changes sign from positive to negative as the temperature decreases. Therefore, the viscosity along an isotherm should first decrease in the vapor phase and subsequently increase with increasing density.<sup>123</sup> Vogel *et al.*<sup>125</sup> have shown that fluids exhibit the same general behavior of the initial density dependence of viscosity, which can also be expressed by means of the second viscosity virial coefficient  $B_\eta(T)$  as

$$B_\eta(T) = \frac{\eta_1(T)}{\eta_0(T)}. \quad (5)$$

The second viscosity virial coefficient can be obtained according to the theory of Rainwater and Friend<sup>10,11</sup> as a function of a reduced second viscosity virial coefficient,  $B_\eta^*(T^*)$ , as

$$B_\eta^*(T^*) = \frac{B_\eta(T)}{N_A \sigma^3}, \quad (6)$$

where<sup>123</sup>

$$B_\eta^*(T^*) = \sum_{i=0}^6 b_i (T^*)^{-0.25i} + b_7 (T^*)^{-2.5} + b_8 (T^*)^{-5.5}. \quad (7)$$

In Eq. (6),  $N_A$  is Avogadro's constant. The coefficients  $b_i$  from Ref. 123 are given in Table 2.

Equations (2)–(7) present a consistent scheme for the correlation of the dilute-gas limit viscosity,  $\eta_0(T)$ , and the initial density dependence term,  $\eta_1(T)$ . In the particular case of *n*-hexane, very accurate dilute-gas limit and initial density dependence viscosity values have been presented by Vogel and Strehlow.<sup>19</sup> These values have been used with the regression package ODRPACK (Ref. 126) in order to fit the coefficients

TABLE 2. Coefficients and parameters for Eqs. (3), (7), and (8)

|                                               |                          |                          |
|-----------------------------------------------|--------------------------|--------------------------|
| Scaling parameters                            |                          |                          |
| $\varepsilon/k_B = 378.4$ K                   | $\sigma = 0.6334$ nm     |                          |
| Coefficients $\alpha_i$ for Eq. (3)           |                          |                          |
| $\alpha_0 = 0.187\ 60$                        | $\alpha_1 = -0.484\ 30$  | $\alpha_2 = 0.044\ 77$   |
| Coefficients $b_i$ for Eq. (7) <sup>123</sup> |                          |                          |
| $b_0 = -19.572\ 881$                          | $b_1 = 219.739\ 99$      | $b_2 = -1015.322\ 6$     |
| $b_3 = 2471.012\ 5$                           | $b_4 = -3375.171\ 7$     | $b_5 = 2491.659\ 7$      |
| $b_6 = -787.260\ 86$                          | $b_7 = 14.085\ 455$      | $b_8 = -0.346\ 641\ 58$  |
| Coefficients $c_i$ for Eq. (8)                |                          |                          |
| $c_0 = 2.534\ 023\ 35$                        | $c_1 = -9.724\ 061\ 002$ | $c_2 = 0.469\ 437\ 316$  |
| $c_3 = 158.557\ 163\ 1$                       | $c_4 = 72.429\ 168\ 56$  | $c_5 = 10.607\ 512\ 53$  |
| $c_6 = 8.628\ 373\ 915$                       | $c_7 = -6.613\ 464\ 41$  | $c_8 = -2.212\ 724\ 566$ |

$\alpha_i$  in Eq. (3) and the scaling parameters  $\sigma$  and  $\varepsilon/k_B$ . The values obtained are shown in Table 2. Figure 3 shows a comparison of the experimental values of  $B_\eta$  from Vogel and Strehlow,<sup>19</sup> along with the values calculated with Eqs. (2)–(7) with the parameters in Table 2. Although Eq. (7) was originally developed for propane, the agreement is quite good. Figure 4 shows a comparison of low-density viscosity data of Vogel and Strehlow<sup>19</sup> with the values calculated with Eqs. (2)–(7). Again, the agreement is good. Based on comparisons with the data of Vogel and Strehlow,<sup>19</sup> we estimate the uncertainty of the correlation for the low-density gas at temperatures from 298 to 631 K to be 0.3%, at a 95% confidence level. Therefore, Eqs. (2)–(7) can be employed for the calculation of the dilute-gas limit viscosity,  $\eta_0(T)$  and the initial density dependence term,  $\eta_1(T)$ .

### 3.2. The critical enhancement term

Viscosity and thermal conductivity of pure fluids diverge at the critical point due to long-range fluctuations. The critical enhancements can be described by a theoretical crossover model originally developed by Olchowy and Sengers<sup>127,128</sup> and modified by Luettmer-Strathmann *et al.*<sup>129</sup> Unlike the

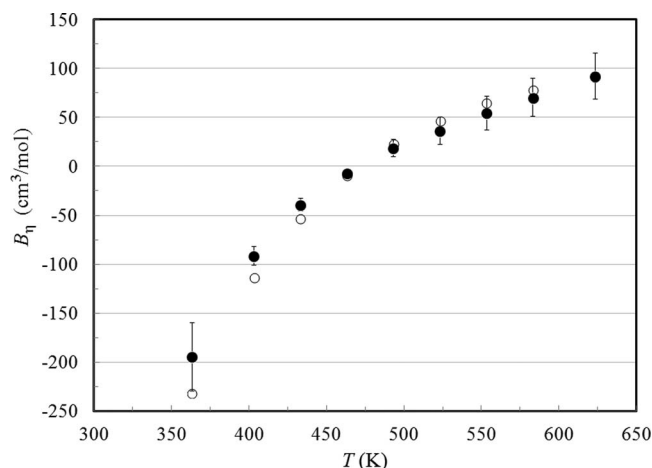


FIG. 3. Comparison of the experimental values of  $B_\eta$  for  $n$ -hexane with values calculated from Eqs. (2)–(7) with the parameters in Table 2. Vogel and Strehlow<sup>19</sup> (●), Eqs. (2)–(7) (○).

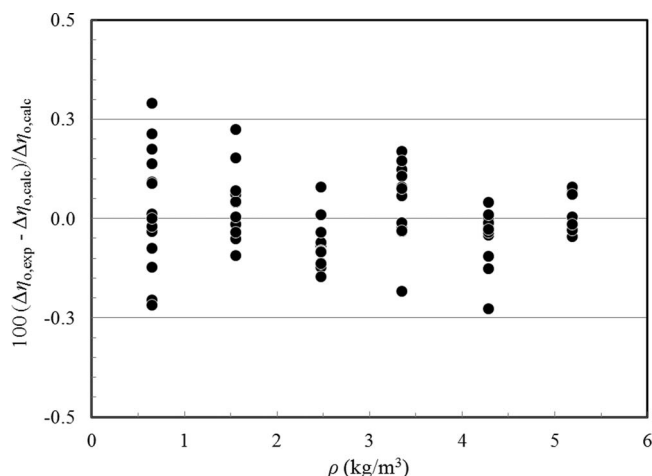


FIG. 4. Percentage deviations of low-density viscosity ( $\Delta\eta_0 = \eta_0 + \eta_1\rho$ ) experimental data of  $n$ -hexane from the values calculated by Eqs. (2)–(7) as a function of the density. Vogel and Strehlow<sup>19</sup> (●).

critical enhancement in thermal conductivity, the enhancement in viscosity is confined to a small region, becoming relevant only at temperatures and densities very close to the critical point. For some fluids,<sup>130,131</sup> the ratio  $\Delta\eta_c(\rho, T)/\eta(\rho, T)$  exceeds 0.01 only within 1% of the critical temperature of the fluid. There are no reliable data for  $n$ -hexane in the critical region. Hence, this contribution is considered negligible and it is not further taken into consideration in this work.

### 3.3. The residual term

As already stated in Sec. 2, the residual viscosity term,  $\Delta\eta(\rho, T)$ , represents the contribution of all other effects to the viscosity of the fluid at elevated densities including many-body collisions, molecular-velocity correlations, and collisional transfer. Because there is little theoretical guidance concerning this term, its evaluation is based entirely on experimentally obtained data.

The procedure adopted during this analysis used symbolic regression software<sup>132</sup> to fit all the primary data to the residual viscosity. Symbolic regression is a type of genetic programming that allows the exploration of arbitrary functional forms to regress data. The functional form is obtained by use of a set of operators, parameters, and variables as building blocks. Most recently, this method has been used to obtain a correlation for the viscosity of hydrogen.<sup>133</sup> In the present work, we restricted the operators to the set (+, −, \*, /) and the operands (constant,  $T_r$ ,  $\rho_r$ ), with  $T_r = T/T_c$  and  $\rho_r = \rho/\rho_c$ . Various choices of a scaling factor for density were tested, but the best results were obtained using the critical density. In addition, we found the best results when we adopted a form suggested from the hard-sphere model employed by Assael *et al.*,<sup>134</sup>  $\Delta\eta(\rho_r, T_r) = (\rho_r^{2/3} T_r^{1/2}) F(\rho_r, T_r)$ , where the symbolic regression method was used to determine the functional form for  $F(\rho_r, T_r)$ . For this task, the dilute-gas limit and the initial density dependence terms were calculated for each experimental point [employing Eqs. (2)–(7)] and subtracted from the experimental viscosity to obtain the residual term. The

TABLE 3. Evaluation of the *n*-hexane viscosity correlation for the primary data

| 1st author              | Year of publication | AAD (%)     | BIAS (%)     |
|-------------------------|---------------------|-------------|--------------|
| Oliveira <sup>14</sup>  | 1992                | 0.83        | −0.11        |
| Assael <sup>15</sup>    | 1991                | 0.80        | −0.79        |
| Berstad <sup>16</sup>   | 1989                | 1.48        | −1.48        |
| Knapstad <sup>17</sup>  | 1989                | 0.78        | −0.78        |
| Grigor'ev <sup>18</sup> | 1988                | 0.61        | −0.23        |
| Vogel <sup>19</sup>     | 1988                | 0.10        | 0.02         |
| Bauer <sup>20</sup>     | 1984                | 1.48        | −1.48        |
| Dymond <sup>21</sup>    | 1980                | 1.05        | 0.36         |
| Dymond <sup>22</sup>    | 1980                | 1.34        | −1.18        |
| Agaev <sup>23 a</sup>   | 1963                | 2.29        | 0.30         |
| <b>Entire data set</b>  |                     | <b>1.56</b> | <b>−0.04</b> |

<sup>a</sup>Excludes data within 0.2 K of the critical temperature and within 0.1 MPa of the critical pressure.

density values employed were obtained by the equation of state of Span and Wagner.<sup>8</sup> The final equation obtained was

$$\Delta\eta(\rho, T) = (\rho_r^{2/3} T_r^{1/2}) \left\{ \frac{c_0}{T_r} + \frac{c_1}{c_2 + T_r + c_3 \rho_r^2} + \frac{c_4(1 + \rho_r)}{c_5 + c_6 T_r + c_7 \rho_r + \rho_r^2 + c_8 \rho_r T_r} \right\}. \quad (8)$$

Coefficients  $c_i$  are given in Table 2.

Table 3 summarizes comparisons of the primary data with the correlation. We have defined the percent deviation as PCTDEV =  $100 \cdot (\eta_{\text{exp}} - \eta_{\text{fit}}) / \eta_{\text{fit}}$ , where  $\eta_{\text{exp}}$  is the experimental value of the viscosity and  $\eta_{\text{fit}}$  is the value calculated from the correlation. Thus, the average absolute percent deviation (AAD) is found with the expression  $\text{AAD} = (\sum |\text{PCTDEV}|) / n$ , where the summation is over all  $n$  points, the bias percent is found with the expression  $\text{BIAS} = (\sum \text{PCTDEV}) / n$ . The average absolute percent deviation of the fit is 1.56, and its bias is −0.04%. We estimate the uncertainty at a 95% confidence level to be 2% for the liquid phase at temperatures up to 450 K and pressures to 100 MPa. For the liquid at 450–600 K, the predominant measurements are those of Agaev and Golubev,<sup>23</sup> which are of higher uncertainty and a larger degree of scatter than other primary data, as indicated in Figs. 2–4. In this region, we estimate the expanded uncertainty at the 95% confidence level to be 6%. As mentioned previously, we estimate the expanded uncertainty of the correlation at a 95% confidence level for the low-density gas at temperatures from 298 to 631 K and pressures to 0.3 MPa to be 0.3%.

Figure 5 shows the percentage deviations of all primary viscosity data from the values calculated by Eqs. (1)–(8) as a function of density, while Figs. 6 and 7 show the same deviations but as a function of the temperature and pressure. With the exception of the data set of Agaev and Golubev,<sup>23</sup> all primary data are represented to within 2% over the temperature range 178–437 K at pressures to 100 MPa with the present model. As already discussed above, the data of Agaev and Golubev<sup>23</sup> display larger deviations. Figure 7 shows the extrapolation behavior above 100–200 MPa. We note that, although the present correlation is restricted to 100 MPa because of the validity of the equation of state, it is the authors'

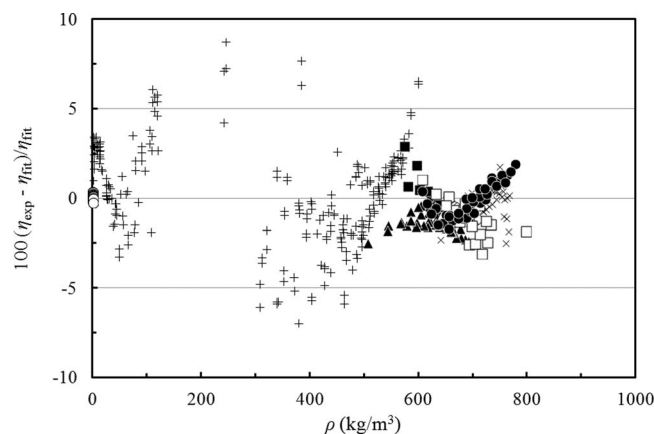


Fig. 5. Percentage deviations of primary experimental data of *n*-hexane from the values calculated by the present model as a function of density. Oliveira and Wakeham<sup>14</sup> (●), Assael *et al.*<sup>15</sup> (◆), Berstad<sup>16</sup> (▲), Knapstad *et al.*<sup>17</sup> (Δ), Grigor'ev *et al.*<sup>18</sup> (×), Vogel and Strehlow<sup>19</sup> (○), Bauer and Mehlender<sup>20</sup> (◆), Dymond and Young<sup>21</sup> (■), Dymond *et al.*<sup>22</sup> (□), Agaev and Golubev<sup>23</sup> (+).

belief that the correlation behaves in a physically reasonable manner at pressures to 500 MPa. However, we estimate that the uncertainties at 500 MPa may be much larger, on the order of 20% to 30%.

In Fig. 6, a previous reference correlation by Dymond and Øye<sup>135</sup> along the saturation line covering the temperature range from 273 to 355 K is also shown. The Dymond and Øye<sup>135</sup> correlation has an uncertainty of 1%, and is in agreement with the present correlation within this uncertainty. The correlation of Dymond and Øye<sup>135</sup> was heavily based on the measurements of Dymond,<sup>21</sup> and also the measurements of Oliveira and Wakeham<sup>14</sup> and Knapstad *et al.*<sup>17</sup> The present correlation includes measurements of additional investigators; see Table 1.

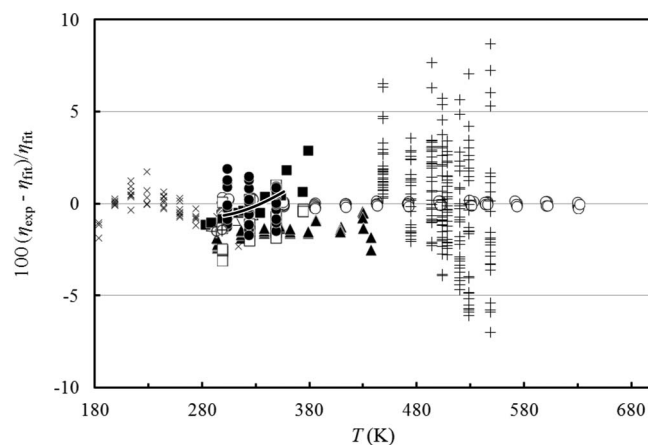


Fig. 6. Percentage deviations of primary experimental data of *n*-hexane from the values calculated by the present model as a function of temperature. Oliveira and Wakeham<sup>14</sup> (●), Assael *et al.*<sup>15</sup> (◆), Berstad<sup>16</sup> (▲), Knapstad *et al.*<sup>17</sup> (Δ), Grigor'ev *et al.*<sup>18</sup> (×), Vogel and Strehlow<sup>19</sup> (○), Bauer and Mehlender<sup>20</sup> (◆), Dymond and Young<sup>21</sup> (■), Dymond *et al.*<sup>22</sup> (□), Agaev and Golubev<sup>23</sup> (+), Dymond and Øye<sup>135</sup> (—).



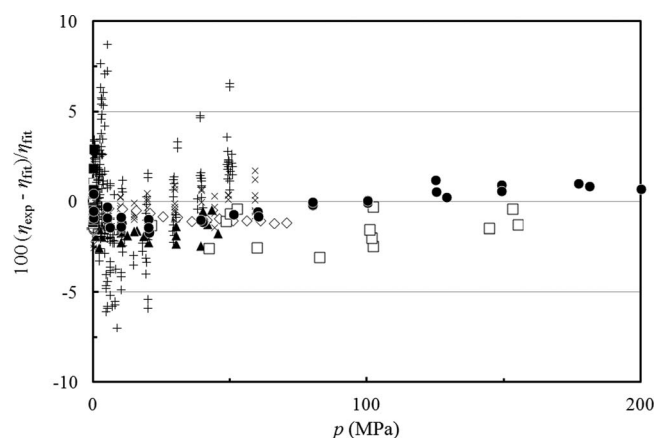


FIG. 7. Percentage deviations of primary experimental data of *n*-hexane from the values calculated by the present model as a function of pressure. Oliveira and Wakeham<sup>14</sup> (●), Assael *et al.*<sup>15</sup> (◆), Berstad<sup>16</sup> (▲), Knapstad *et al.*<sup>17</sup> (Δ), Grigor'ev *et al.*<sup>18</sup> (×), Vogel and Strehlow<sup>19</sup> (○), Bauer and Mehlender<sup>20</sup> (♦), Dymond and Young<sup>21</sup> (■), Dymond *et al.*<sup>22</sup> (□), Agaev and Golubev<sup>23</sup> (+).

Quiñones-Cisneros and Deiters<sup>136</sup> published a wide-ranging viscosity model based on friction theory applied to several fluids, including *n*-hexane. Figures 8–10 show percentage deviations of the primary data calculated with this friction-theory model as a function of the density, the temperature and the pressure, using the same equation of state as was used for the present model (the short Span-Wagner<sup>8</sup> EOS). The comparisons with the friction theory model indicate that it has similar performance to the present model except for the low-temperature ( $T < \sim 270$  K) high-density region. This is not surprising considering that the *n*-hexane friction-theory model presented is very general, did not incorporate the 1988 data set of Grigor'ev *et al.*,<sup>18</sup> and was not developed specifically for *n*-hexane.

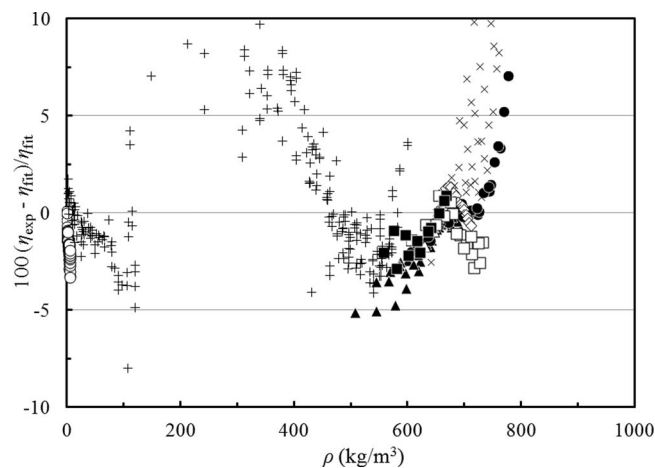


FIG. 8. Percentage deviations of primary experimental data of *n*-hexane from the values calculated by the friction-theory model as a function of density. Oliveira and Wakeham<sup>14</sup> (●), Assael *et al.*<sup>15</sup> (◆), Berstad<sup>16</sup> (▲), Knapstad *et al.*<sup>17</sup> (Δ), Grigor'ev *et al.*<sup>18</sup> (×), Vogel and Strehlow<sup>19</sup> (○), Bauer and Mehlender<sup>20</sup> (♦), Dymond and Young<sup>21</sup> (■), Dymond *et al.*<sup>22</sup> (□), Agaev and Golubev<sup>23</sup> (+).

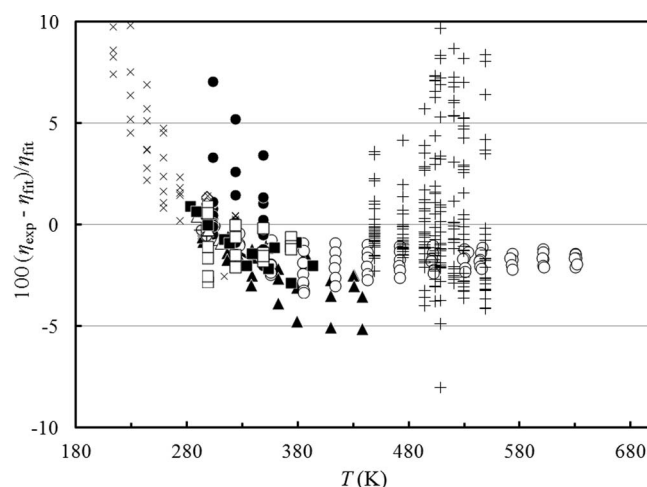


FIG. 9. Percentage deviations of primary experimental data of *n*-hexane from the values calculated by the friction-theory model as a function of temperature. Oliveira and Wakeham<sup>14</sup> (●), Assael *et al.*<sup>15</sup> (◆), Berstad<sup>16</sup> (▲), Knapstad *et al.*<sup>17</sup> (Δ), Grigor'ev *et al.*<sup>18</sup> (×), Vogel and Strehlow<sup>19</sup> (○), Bauer and Mehlender<sup>20</sup> (♦), Dymond and Young<sup>21</sup> (■), Dymond *et al.*<sup>22</sup> (□), Agaev and Golubev<sup>23</sup> (+), Dymond and Øye<sup>135</sup> (–).

In Table 4, values are given along the saturation line, calculated from the proposed correlation between 250 and 350 K. The uncertainty of these values is 2% at the 95% confidence level. Table 5 shows the AAD and the bias for the secondary data. Finally, Fig. 11 shows a plot of the viscosity of *n*-hexane as a function of the temperature for different pressures.

#### 4. Computer-Program Verification

Table 6 is provided to assist the user in computer-program verification. The viscosity calculations are based on the tabulated temperatures and densities.

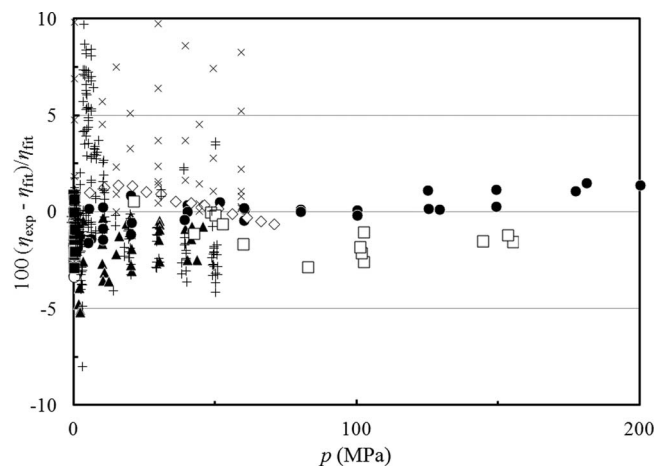


FIG. 10. Percentage deviations of primary experimental data of *n*-hexane from the values calculated by the friction-theory model as a function of pressure. Oliveira and Wakeham<sup>14</sup> (●), Assael *et al.*<sup>15</sup> (◆), Berstad<sup>16</sup> (▲), Knapstad *et al.*<sup>17</sup> (Δ), Grigor'ev *et al.*<sup>18</sup> (×), Vogel and Strehlow<sup>19</sup> (○), Bauer and Mehlender<sup>20</sup> (♦), Dymond and Young<sup>21</sup> (■), Dymond *et al.*<sup>22</sup> (□), Agaev and Golubev<sup>23</sup> (+).

TABLE 4. Viscosity values of the liquid along the saturation line, calculated by the present scheme

| <i>T</i> (K) | $\rho$ (kg m <sup>-3</sup> ) | $\eta$ (μPa s) |
|--------------|------------------------------|----------------|
| 250.00       | 697.89                       | 514.4          |
| 260.00       | 689.05                       | 452.7          |
| 270.00       | 680.16                       | 401.8          |
| 280.00       | 671.19                       | 359.2          |
| 290.00       | 662.14                       | 323.1          |
| 300.00       | 652.98                       | 292.1          |
| 310.00       | 643.70                       | 265.2          |
| 320.00       | 634.26                       | 241.7          |
| 330.00       | 624.66                       | 221.0          |
| 340.00       | 614.86                       | 202.6          |
| 350.00       | 604.84                       | 186.2          |

TABLE 5. Evaluation of the *n*-hexane viscosity correlation for the secondary data

| 1st author               | Year of publication | AAD (%) | BIAS (%) |
|--------------------------|---------------------|---------|----------|
| Guerrero <sup>24</sup>   | 2011                | 2.29    | 0.50     |
| Rathnam <sup>25</sup>    | 2010                | 0.84    | 0.03     |
| Dominguez <sup>26</sup>  | 2009                | 0.73    | 0.73     |
| Feitosa <sup>27</sup>    | 2009                | 4.06    | -4.06    |
| Sastry <sup>28</sup>     | 2009                | 1.72    | 0.32     |
| Bandres <sup>29</sup>    | 2008                | 0.83    | 0.14     |
| Fang <sup>30</sup>       | 2008                | 3.00    | 3.00     |
| Shukla <sup>31</sup>     | 2008                | 0.47    | -0.47    |
| Dubey <sup>32</sup>      | 2007                | 6.05    | 6.05     |
| Reddy <sup>33</sup>      | 2007                | 10.02   | 10.02    |
| Tian <sup>34</sup>       | 2007                | 2.19    | 1.51     |
| Kumagai <sup>35</sup>    | 2006                | 1.29    | -0.55    |
| Baragi <sup>36</sup>     | 2006                | 4.69    | 4.69     |
| Iloukhani <sup>37</sup>  | 2006                | 1.64    | -1.20    |
| Modarress <sup>38</sup>  | 2006                | 1.23    | 1.23     |
| Rodriguez <sup>39</sup>  | 2006                | 0.63    | 0.55     |
| Al-Jimaz <sup>40</sup>   | 2005                | 0.70    | 0.70     |
| Tripathi <sup>41</sup>   | 2005                | 0.40    | -0.40    |
| Yang <sup>42</sup>       | 2004                | 1.35    | -1.22    |
| Bolotnikov <sup>43</sup> | 2003                | 5.23    | 5.23     |
| Dominguez <sup>44</sup>  | 2003                | 0.41    | -0.41    |
| Nayak <sup>45</sup>      | 2003                | 6.69    | 6.69     |
| Oswal <sup>46</sup>      | 2003                | 0.91    | -0.91    |
| Comelli <sup>47</sup>    | 2002                | 0.05    | -0.05    |
| Garcia <sup>48</sup>     | 2002                | 12.59   | 12.59    |
| Peng <sup>49</sup>       | 2002                | 0.63    | 0.63     |
| Chowdhury <sup>50</sup>  | 2001                | 3.12    | 3.12     |
| Gascon <sup>51</sup>     | 2001                | 0.02    | 0.01     |
| Postigo <sup>52</sup>    | 2001                | 1.93    | 1.22     |
| Tu <sup>53</sup>         | 2001                | 2.31    | 2.31     |
| Lal <sup>54</sup>        | 2000                | 0.39    | -0.39    |
| Aralaguppi <sup>55</sup> | 1999                | 2.31    | 2.31     |
| Barnes <sup>56</sup>     | 1999                | 7.43    | -7.43    |
| Casas <sup>57</sup>      | 1998                | 1.41    | -1.41    |
| Aminabhavi <sup>58</sup> | 1997                | 1.49    | 1.49     |
| Nath <sup>59</sup>       | 1997                | 0.74    | -0.74    |
| Orge <sup>60</sup>       | 1997                | 6.72    | 6.72     |
| Sastry <sup>61</sup>     | 1996                | 1.20    | 1.20     |

TABLE 5. Evaluation of the *n*-hexane viscosity correlation for the secondary data—Continued

| 1st author                  | Year of publication | AAD (%) | BIAS (%) |
|-----------------------------|---------------------|---------|----------|
| Aucejo <sup>62</sup>        | 1995                | 1.20    | 1.20     |
| Franjo <sup>63</sup>        | 1995                | 3.07    | -3.07    |
| Rived <sup>64</sup>         | 1995                | 1.33    | -1.33    |
| Papaioannou <sup>65</sup>   | 1994                | 4.00    | -3.93    |
| De Lorenzi <sup>66</sup>    | 1994                | 0.37    | 0.37     |
| Kiran <sup>67</sup>         | 1992                | 2.89    | 2.64     |
| Cooper <sup>68</sup>        | 1991                | 0.00    | 0.00     |
| Abdelrazig <sup>69</sup>    | 1990                | 65.89   | 65.89    |
| Chevalier <sup>70</sup>     | 1990                | 1.40    | -1.40    |
| Iwahashi <sup>71</sup>      | 1990                | 6.26    | 6.26     |
| Sekar <sup>72</sup>         | 1990                | 13.94   | 13.94    |
| Grachev <sup>73</sup>       | 1989                | 4.51    | -3.03    |
| Schrodt <sup>74</sup>       | 1989                | 2.86    | 2.86     |
| Chandrasekhar <sup>75</sup> | 1988                | 0.80    | -0.80    |
| Rao <sup>76</sup>           | 1988                | 10.79   | 10.79    |
| Awad <sup>77</sup>          | 1986                | 4.89    | 4.89     |
| Craubner <sup>78</sup>      | 1986                | 0.16    | -0.16    |
| Singh <sup>79</sup>         | 1985                | 0.13    | -0.13    |
| Singh <sup>80</sup>         | 1984                | 8.34    | 8.34     |
| Wei <sup>81</sup>           | 1984                | 2.04    | -2.04    |
| Kashiwagi <sup>83</sup>     | 1982                | 0.74    | -0.64    |
| Sreenivasulu <sup>82</sup>  | 1982                | 1.03    | -1.03    |
| Asfour <sup>84</sup>        | 1981                | 0.33    | -0.33    |
| Teja <sup>85</sup>          | 1981                | 0.74    | -0.13    |
| Isdale <sup>86</sup>        | 1979                | 10.06   | -9.12    |
| Gouel <sup>87</sup>         | 1978                | 3.76    | -1.14    |
| Medani <sup>88</sup>        | 1977                | 4.89    | -0.97    |
| Bulanov <sup>89</sup>       | 1975                | 2.83    | 2.55     |
| Diaz Pena <sup>90</sup>     | 1975                | 5.47    | 5.47     |
| Moore <sup>91</sup>         | 1974                | 0.49    | 0.41     |
| Strumpf <sup>92</sup>       | 1974                | 2.05    | 2.05     |
| Naziev <sup>93</sup>        | 1972                | 2.70    | -0.93    |
| Eicher <sup>94</sup>        | 1972                | 0.47    | 0.38     |
| Heric <sup>95</sup>         | 1972                | 0.13    | 0.13     |
| Ghai <sup>96</sup>          | 1971                | 0.17    | 0.17     |
| Ratcliff <sup>97</sup>      | 1971                | 0.24    | 0.24     |
| Brazier <sup>98</sup>       | 1969                | 2.51    | 1.72     |
| Kuss <sup>99</sup>          | 1969                | 1.31    | -1.20    |
| Johari <sup>100</sup>       | 1968                | 1.13    | -1.13    |
| Diaz Pena <sup>101</sup>    | 1967                | 2.31    | -0.57    |
| Ridgway <sup>102</sup>      | 1967                | 3.14    | -3.14    |
| Parisot <sup>103</sup>      | 1961                | 1.84    | 1.84     |
| Reed <sup>104</sup>         | 1959                | 0.86    | -0.86    |
| Lambert <sup>105</sup>      | 1955                | 5.63    | 5.63     |
| Cummings <sup>106</sup>     | 1952                | 2.90    | -1.90    |
| Craven <sup>107</sup>       | 1951                | 8.12    | 8.12     |
| McCoubrey <sup>108</sup>    | 1951                | 1.01    | 1.01     |
| Grunberg <sup>109</sup>     | 1950                | 4.91    | 4.91     |
| Giller <sup>110</sup>       | 1949                | 3.55    | -3.55    |
| Geist <sup>111</sup>        | 1946                | 0.73    | -0.73    |
| Khalilov <sup>112</sup>     | 1939                | 11.80   | -2.10    |
| Andrade <sup>113</sup>      | 1936                | 2.91    | 2.91     |
| Titani <sup>114</sup>       | 1933                | 13.70   | -12.07   |
| Shepard <sup>115</sup>      | 1931                | 0.50    | -0.50    |
| Timmermans <sup>116</sup>   | 1928                | 0.45    | 0.22     |
| Bridgman <sup>117</sup>     | 1926                | 5.39    | 5.39     |
| Batschinski <sup>118</sup>  | 1913                | 3.28    | 3.28     |
| Drapier <sup>119</sup>      | 1911                | 2.30    | 2.30     |
| Thorpe <sup>120</sup>       | 1894                | 3.30    | 3.30     |

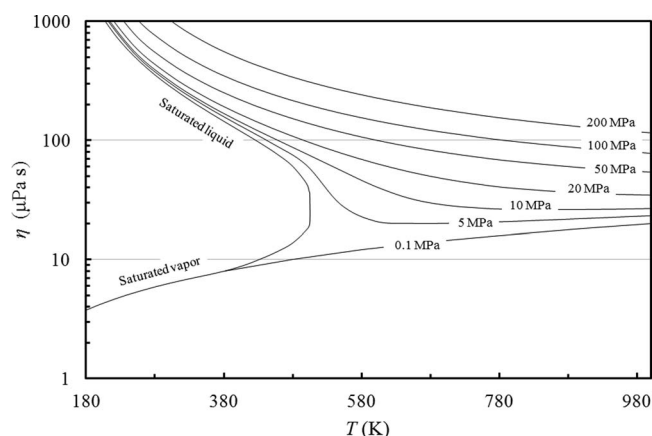


FIG. 11. Viscosity of *n*-hexane as a function of temperature for selected pressures.

TABLE 6. Sample points for computer verification of the correlating equations

| <i>T</i> (K) | $\rho$ (kg m <sup>-3</sup> ) | $\eta$ (μPa s) |
|--------------|------------------------------|----------------|
| 250.00       | 0.00                         | 5.2584         |
| 400.00       | 0.00                         | 8.4149         |
| 550.00       | 0.00                         | 11.442         |
| 250.00       | 700.00                       | 528.20         |
| 400.00       | 600.00                       | 177.62         |
| 550.00       | 500.00                       | 95.002         |

## 5. Conclusion

A new wide-ranging correlation for the viscosity of *n*-hexane was developed based on critically evaluated experimental data. The correlation is valid from the triple point to 600 K, and at pressures up to 100 MPa. The correlation is expressed in terms of temperature and density, with the density calculated from the equation of state of Span and Wagner.<sup>8</sup> The average absolute percent deviation of the fit is 1.56%, with bias  $-0.04\%$ . We estimate the expanded uncertainty at a 95% confidence level to be 2% for the liquid phase at temperatures up to 450 K and pressures to 100 MPa. For the liquid at 450–600 K at pressures to 100 MPa, the expanded uncertainty at the 95% confidence level is 6%, and is 0.3% for the low-density gas at temperatures from 298 to 631 K and pressures to 0.3 MPa.

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