Online Data Resources in Chemical Engineering Education:
IMPACT OF THE UNCERTAINTY CONCEPT FOR THERMOPHYSICAL PROPERTIES[1,2]

Sun Hyung Kim and Jeong Won Kang
Korea University • Seoul, Korea
Kenneth Kroenlein, Joseph W. Magee, Vladimir Diky,
Chris D. Muzny, Andrei F. Kazakov, Robert D. Chirico, and Michael Frenkel
Thermophysical Properties Division, National Institute of Standards and Technology • Boulder, CO 80305-3337

While the analysis of uncertainty has long been recognized as one of the cornerstones of measurement science, its practical implementation in a variety of scientific and engineering fields has typically seen less emphasis than it deserves. This is particularly true for the field of thermodynamics, which deals with more than 120 thermophysical and thermochemical properties that are of paramount importance for the support of both the scientific discovery process and a great number of large-scale industrial applications. This point was clearly demonstrated by recent study[1] conducted by the Thermodynamics Research Center (TRC) of the U.S. National Institute of Standards and Technology (NIST), which involved a review of reporting practices for uncertainty in the literature. Establishment of a global communication process in the field of thermodynamics[2] that involves NIST/TRC and five journals in the field (*Journal of Chemical and Engineering Data*, *Journal of Chemical Thermodynamics*, *Fluid Phase Equilibria*, *Thermochimica Acta*, and the *International Journal of Thermophysics*) has led to the finding that at least 10% of articles reporting measurement of thermodynamic properties contain some erroneous information in numerical data and/or metadata. These findings demonstrated, again, the necessity for unambiguous reporting of uncertainties for all experimental data in order to aid the process of data validation. This has led to new requirements

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Sun Hyung Kim *received a B.S. from Korea University in 2008 in chemical engineering. He is currently a graduate student under the guidance of Professor Jeong Won Kang in the Department of Chemical and Biological Engineering, Korea University.*

Jeong Won Kang *received a B.S., M.S., and Ph.D. from Korea University in 1988, 1990, and 2001, all in chemical engineering. He worked at Hyundai Engineering Co. Ltd. from 1990 to 1997. He is currently an associate professor in the Department of Chemical and Biological Engineering, Korea University. His research has been mainly focused on measurements and model development for thermophysical properties of fluids.*

Kenneth Kroenlein *received a B.S.E. and Ph.D. from Princeton University in 2001 and 2007, respectively, both in mechanical and aerospace engineering. He is currently a mechanical engineer with the National Institute of Standards and Technology. His research has been mainly focused on thermophysical property evaluation, cheminformatics, and combustion phenomena.*

Joseph W. Magee *received a B.S. in 1978 from Georgia Institute of Technology, and an M.S.(1981) and Ph.D.(1983) from Rice University, all in chemical engineering. He is currently a chemical engineer with the National Institute of Standards and Technology. He has held engineering faculty adjoint/guest appointments at CU-Boulder and NDA (Yokosuka, Japan). His research interests are in the areas of thermodynamic property measurements and data analysis/evaluation.*

Vladimir Diky *received M.S. and Ph.D. degrees from Belarusian State University (Belarus) in 1990 and 1993, respectively. He is currently a chemist at the National Institute of Standards and Technology. His principal research interests include analysis and modeling of thermodynamic data, communication of chemical information, and chemical process simulation.*

Chris D. Muzny *received a B.S. in 1982 from Southeastern Oklahoma State University in physics and mathematics, and an M.S.(1986) and Ph.D.(1994) in physics from the University of Colorado at Boulder. He is currently a physicist at the National Institute of Standards and Technology. He works for the Thermodynamics Research Center on the development and maintenance of a database of thermophysical properties of a large range of mostly hydrocarbon substances.*

Andrei F. Kazakov *received an M.S. in 1989 from Moscow Institute of Physics and Technology (Russia) and a Ph.D. in 1997 from Pennsylvania State University. He is currently a physicist with the National Institute of Standards and Technology. His research is in the areas of combustion physics and modeling of thermodynamic properties.*

Robert D. Chirico *received an A.B. in chemistry from Rutgers University in 1974, and a Ph.D. in chemistry at the University of Michigan in 1979. He is currently a chemist with the National Institute of Standards and Technology. His research is in the areas of thermodynamic property measurements and data analysis/evaluation.*

Michael Frenkel *received an M.S. in chemistry from Belarusian State University (Belarus) in 1975 and a Ph.D. in Physical Chemistry in 1981 from the same university. Currently, he is director of the Thermodynamics Research Center at the National Institute of Standards and Technology (Boulder, Colorado). His research interests include phenomenological and statistical thermodynamics, molecular modeling, and software expert systems.*

for mandatory provision of combined uncertainties within data tables.[3-8] As recently demonstrated,[9] inadequate, incomplete, or missing uncertainty information for experimental data can, in turn, lead to poorly developed structure-property correlations. A lack of reliable estimates of uncertainties for thermophysical property data commonly results in overdesign of production modules in chemical manufacturing with an associated enormous waste of energy and materials.[10-11]

In the long term, we believe that undergraduate and graduate-level educational institutions are the key venues in which to address the issues associated with poor understanding of the concept of uncertainties for physical properties. Until very recently, however, progress has been limited, to a significant degree, due to the absence of resources providing comprehensively assessed uncertainties of critically evaluated data. Recent development and software implementation of the concepts of a Global Information System in Science with application to the field of thermodynamics[12] and of dynamic data evaluation for thermophysical and thermochemical properties[13-18] in combination with modern Web technologies for data communication[19] now provide a unique opportunity to bring state-of-the-art metrology to the classroom for a new generation of chemical engineers. This article presents an overview of the technical background and basic concepts of propagated uncertainties, plus a summary of online data resources for thermophysical and thermochemical properties, and then illustrates how the concept of uncertainties for properties can be brought to the curriculum of traditional chemical engineering courses, such as thermodynamics and chemical process design, with the use of the available online data resources.

UNCERTAINTIES OF THERMOPHYSICAL AND THERMOCHEMICAL PROPERTIES

Efforts to provide guidance in the assessment of uncertainty as a foundation for measurement science date back to the 1970s. Those efforts resulted in the publication of the *Guide to the Expression of Uncertainty in Measurement*[20] in 1993. These ISO (International Organization for Standardization) recommendations were adopted with minor changes as the *U.S. Guide to the Expression of Uncertainty in Measurement*.[21] Reference 20 is commonly referred to by its abbreviation, the *GUM*. The *GUM* recommendations have been summarized in *Guidelines for the Evaluation and Expression of Uncertainty in NIST Measurement Results*,[22] which is available via free download from the Web.[23] The *GUM* provides definitions of all quantities and terms relevant to uncertainty, but by design, does not provide their interpretation for specific scientific and engineering fields. The *GUM* concepts were further interpreted for the field of thermodynamics in 2003[24] by an IUPAC (International Union for Pure and Applied Chemistry) Task Group as a part of the IUPAC project 2002-055-3-024 "XML-based IUPAC Standard for Experimentally and Critically Evaluated Thermodynamic Property Data Storage and Capture."[25] This interpretation has now become a part of the IUPAC standard for thermophysical and thermochemical property data communication, ThermoML.[26] ThermoML was first adopted by IUPAC in 2006[27] and was further extended in 2011.[28]

In compliance with the recommendations of the *GUM* and in accordance with the provisions of ThermoML, various forms of *precision* such as *repeatability, root-mean-square (rms) deviation from a fitted curve (for a data set)*, and *measuring device specification* can be used to partially characterize data quality for components of the metadata infrastructure of thermophysical and thermochemical properties data (*i.e.*, properties, variables, and constraints).

The only comprehensive measure of overall data quality, however, is the combined expanded uncertainty. Basic principles, definitions of terms and interpretation of the combined expanded uncertainty for thermodynamic quantities have been described in detail.[25] The quantity combined expanded uncertainty reflects all possible sources of error associated with propagated uncertainties for variables and constraints, as well as in the case of experimental data, those related to sample purity and quality of the measuring device, and in case of predicted data, those related to the nature of the prediction model. Combined expanded uncertainties for thermophysical and thermochemical properties are usually provided with the coverage factor (multiplier of standard uncertainty) of 2, which is associated with a level of confidence of 95%.

Critically evaluated data are recommended property values generated through assessment of available experimental and predicted data and their uncertainties.[13] Based on the analysis above, it is clear that critically evaluated data, supplemented with their combined expanded uncertainties, are the most reliable information to be used in applications requiring thermophysical and thermochemical property data.

THERMOPHYSICAL AND THERMOCHEMICAL PROPERTY DATA RESOURCES

The evolution of data resources for thermophysical and thermochemical properties (from hard-copy to main-frame to PC to relational data facilities to the Web) has been discussed recently by Frenkel.[29] Currently, there are several of high-quality data resources available online on a subscription basis (DECHEMA,[30] PPDS,[31] DIPPR[32]) or through response-upon-availability query (Dortmund Data Bank).[33] Generally, all of these resources provide some assessment of the quality of the data.

The recently developed NIST Web Thermo Tables (WTT),[19,34] also available on a subscription basis, provide critically evaluated thermophysical and thermochemical property data for pure compounds. A unique feature of WTT is the characterization of each property value with a

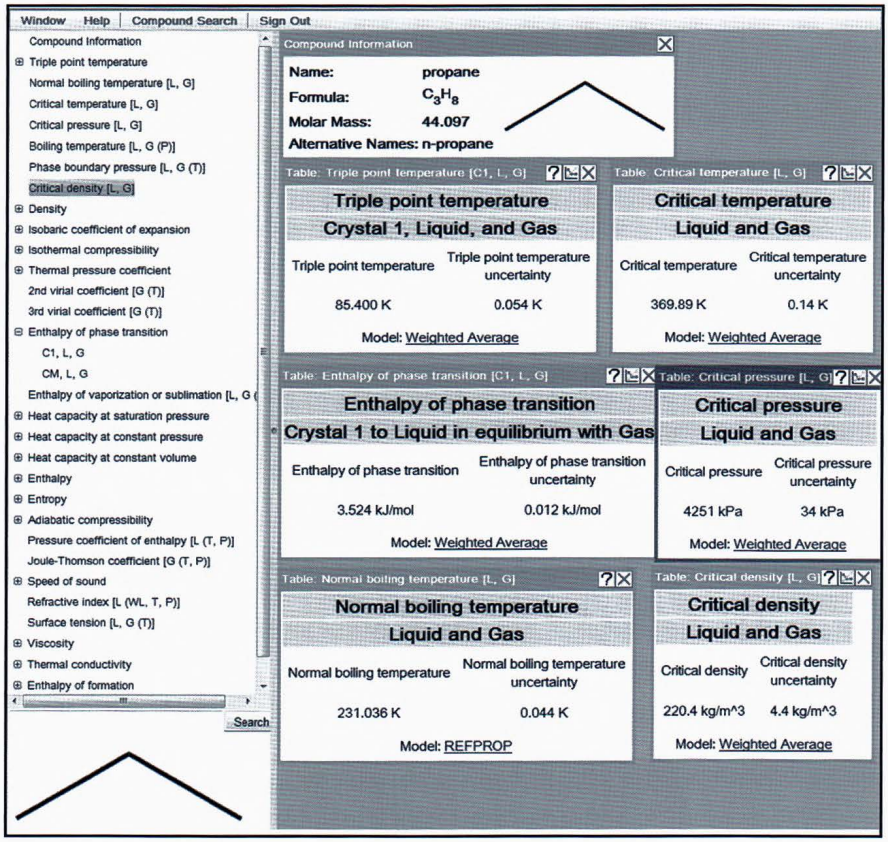
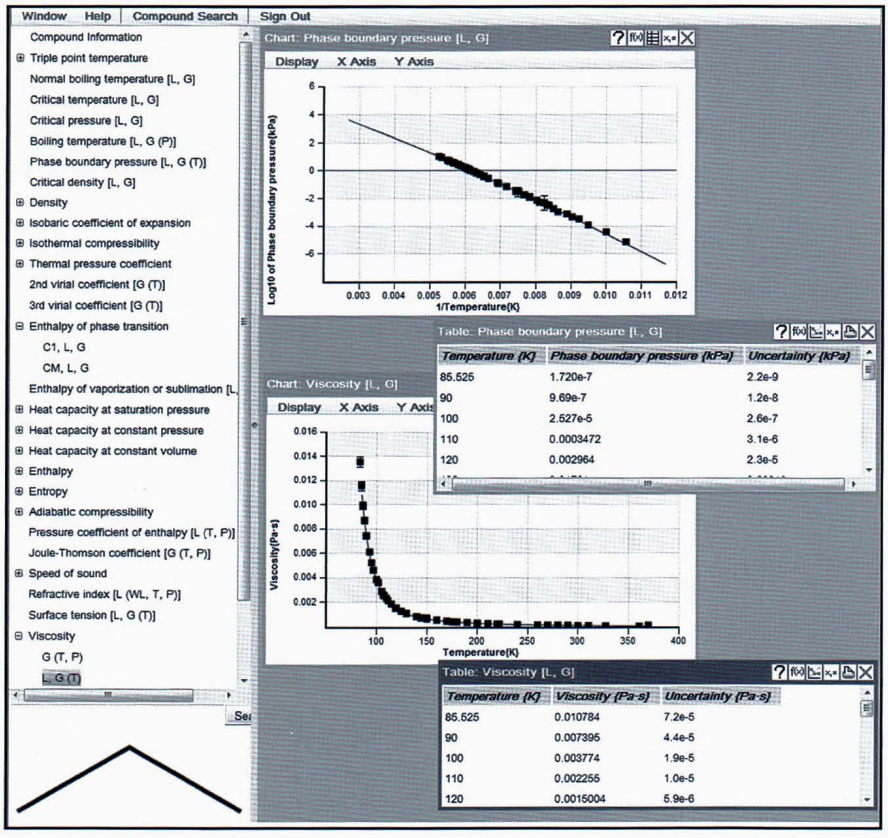


Figure 1. *Example of invariant properties for propane extracted from WTT.*



combined expanded uncertainty. WTT is a Web application of the NIST ThermoData Engine (TDE)[13-18,35] with a Professional Edition (covering 23,399 compounds as of November 2011) and a Lite Edition (covering most common 150 compounds).[34] TDE represents the first full-scale software implementation of the dynamic data evaluation concept. This concept requires large electronic databases capable of storing essentially all relevant experimental data known to date, with detailed descriptions of metadata and uncertainties. The combination of these electronic databases with expert-system software, designed to automatically generate recommended property values based on available experimental and predicted data, leads to the ability to furnish critically evaluated data dynamically or "to order."[12]

WTT includes a system for caching evaluation results to maintain high availability and an advanced window-in-window interface that leverages modern Web-browser technologies[19] with full traceability to the original sources of information. WTT provides a variety of critically evaluated thermodynamic property data for pure components, including phase-diagram, volumetric, energy-related, and transport properties. While WTT is limited currently to pure compounds, its extension to binary mixtures, ternary mixtures, and chemical reactions based on TDE software libraries is expected in the near future. Since WTT provides critically evaluated data with assigned combined expanded uncertainties, it provides a unique opportunity to illustrate the uncertainty concept in traditional courses of the chemical engineering curriculum. Examples of extraction from WTT of invariant and variable-dependent thermophysical properties, plus their uncertainties, for propane are provided in Figures 1 and 2.

Figure 2 (left). *Examples of temperature-dependent properties (saturated vapor pressure and liquid viscosity) for propane extracted from WTT. Vapor pressures are plotted on a logarithmic scale, as a function of reciprocal temperature.*

USE OF WTT FOR EDUCATIONAL PURPOSES —THERMODYNAMICS COURSES

Thermodynamics is one of the fundamental courses in the curriculum for students majoring in chemistry, mechanical engineering, and chemical engineering. In-depth understanding of thermophysical and thermochemical properties is critical for adequate progress in learning essentially all principal topics in the chemical engineering curriculum (First and Second Laws, power cycles, steam engines and turbines, fluid flow, refrigeration, generalized p-V-T relations, the standard Gibbs energy concept, etc.). This understanding lays a firm foundation for their extensive use in other courses of the chemical engineering curriculum and supports a unified approach to consideration of flow processes, power generation, compression of gases, chemical equilibria, fluid flow, heat balances, etc.[36] None of these topics can be satisfactorily analyzed without state-of-the-art knowledge based on the concept of the combined expanded uncertainty as the fundamental measure of reliability of thermophysical and thermochemical properties. No one part of this information is more or less important than others. In fact, numerical value, combined expanded uncertainty, and metadata infrastructure (phases, variables, constraints, units) are equally important and essential for appropriate use of property data for educational purposes in a thermodynamics course. The use of WTT provides the opportunity for students to analyze a broad variety of materials outside of commonly used examples, such as water, air, and refrigerants.

Two examples, similar to those provided in the textbook of Smith et al.,[37] and fully described in the appendix (Appendix 1), provide a comparison of two calculations of molar volume for ethylene (with its combined expanded uncertainty) at a given temperature and pressure. In the first example, a three-term virial equation of state is used, and in the second, the critically evaluated density of the gas is applied. The identical results obtained illustrate that WTT technology enforces thermodynamic consistency between the related properties within their uncertainties.

USE OF WTT FOR EDUCATIONAL PURPOSES —PROCESS DESIGN AND OTHER CORE COURSES

Core courses in chemical engineering—such as elementary process calculations, fluid mechanics, heat and mass transfer, reaction engineering, conceptual design, process simulation, and process control—require knowledge of a variety of thermophysical properties to illustrate key concepts involved. A process-design course, in many ways, integrates knowledge from a number of core chemical engineering courses. In taking full advantage of computing capability and multimedia support for self-paced instruction, Lewin et al.[38] emphasized that presently, early-career chemical engineers are expected to improve product quality, while at the same time reducing operating costs and environmental impact, improving operability, minimizing waste production, and eliminating hazards. It is, therefore, incumbent on chemical engineering educators to provide a modern curriculum for process design instruction that addresses these needs, while being mindful of time constraints.[38] It is critical, in our view, that this instruction would include sufficient focus on uncertainties of thermophysical properties and their impact on decision-making including selection of process technology, flowsheet, and its operating parameters, particularly with regard to emerging interests in energy and sustainability.[39] Indeed, for example, Larsen[10] showed that a 20% error in density may result in a 16% change in equipment size (or cost), and a 20% error in diffusivity may result in a 4% error in equipment size.

Successful efforts in teaching chemical process design are impossible without extensive use of process simulators. Recently,[40,41] the elements of the NIST ThermoData Engine[35] were integrated into process simulation software. That development provides an opportunity to analyze the impact of uncertainty in thermophysical properties on characteristics and cost of principal operation units through commercial process simulators, such as Aspen Plus.[42] This is not possible to do online, however, which must be considered when taking into account time limitations. Similarly, various chemical product design applications of the ThermoData Engine technology are currently available only in the stand-alone format.[17] Consequently, WTT presents a unique opportunity to illustrate the impact of uncertainty of thermophysical properties on engineering applications within the core chemical engineering courses.

The example provided in the Appendix 2 is similar to that in the textbook by Denn[43] and illustrates propagation of uncertainties in a pipe-sizing calculation. The results obtained show that the impact of uncertainty in density on the pipe diameter is much higher than that of the uncertainty in viscosity. Fortunately, densities are usually reported with smaller uncertainties than viscosities, but this cannot be assumed.

The example discussed in the Appendix 3 is similar to that in the textbook by Incropera et al.[44] and illustrates the impact of the combined uncertainty of the thermophysical properties on design of a pipe-inside-pipe heat exchanger. This example shows that the properties of the hot-side stream are of utmost importance when considering the appropriate length of the heat exchanger. It also shows that, in principle, disregarding uncertainties in thermophysical properties of the process streams may lead to serious problems in designing process unit operations.

USE OF ONLINE DATA RESOURCES FOR UNDERGRAD AND GRAD RESEARCH

As a comprehensive online resource for thermophysical property data with combined expanded uncertainties, WTT can be used extensively in graduate and undergraduate re-

search in chemical engineering, targeting the development of new and modification of existing chemical processes. It can also be used in development and verification of property models and correlations using large data sets with uncertainties as a measure of their reliability. Finally, graduate and undergraduate students can use ThermoPlan,[45] a public domain, free-access, online software product, to develop their plans for experimental measurements of thermophysical properties. Specifically, ThermoPlan is a software tool for assistance in the process of experiment planning for thermophysical property measurements. As it was for WTT, ThermoPlan was also developed with ThermoData Engine technology, in part, to respond to the increasing need of the scientific and engineering communities for experiment planning in the field of thermophysical property measurement science, which is envisioned to undergo the transformation "from accuracy to fitness for purpose."[46] ThermoPlan provides recommendations concerning the relative merit of a given measurement via assessment of the existing body of knowledge, including availability of experimental thermophysical property data, associated uncertainties, variable ranges studied, state of prediction methods, and availability of parameters for deployment of prediction methods.

CONCLUSIONS

Themophysical-property data continue to be key and fundamental to chemical engineering education and research. The concept of uncertainty of thermophysical property data cannot be overlooked and is of increasingly high importance. The availability of online resources of thermophysical properties has permanently changed the landscape in both education and research. We believe that these new opportunities should not be lost and that extensive use of the concept of the combined expanded uncertainty for thermophysical and thermochemical properties in thermodynamics courses, as well as in other core courses of the chemical engineering curriculum, including chemical process design, is paramount to ensure that the new generation of chemical engineers will be able to respond to modern challenges in designing new chemical products and processes.

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APPENDIX 1: EXAMPLE FOR A THERMODYNAMICS COURSE

Problem:

Calculate molar volume (V) and its uncertainty for ethylene at 25 °C and 12 bar, with two solutions, designated by (a) and (b):

(a) by using the truncated (three terms) virial equation of state given by,

$$Z = 1 + \frac{B}{V} + \frac{C}{V^2}, \tag{1}$$

where Z is the compressibility factor, and B and C are the second and the third virial coefficients; and, (b) derived from the critically evaluated density in the gas state.

Solution:

$T = 25\ ^\circ C = 298.15\ K, P = 12\ bar = 1.2\times10^6\ Pa, R = 8.314462\ J\cdot mol^{-1}\cdot K^{-1}$

(a) Values of virial coefficients are calculated from WTT at a given temperature (see Figure 3, next page),

$B = (-1.401 \pm 0.042) \times 10^{-4}\ m^3\cdot mol^{-1}$ and $C = (7.47 \pm 0.37) \times 10^{-9}\ m^6\cdot mol^{-2}$,

$$Z = \frac{PV}{RT} = 1 + \frac{B}{V} + \frac{C}{V^2}, \tag{2}$$

Numerical solution of the above equations with given constants yields

$V = 1.91918 \times 10^{-3}\ m^3\cdot mol^{-1}$. Combined expanded uncertainty is given by

$$u_v^2 = \left(\frac{\partial V}{\partial B}\right)^2 u_B^2 + \left(\frac{\partial V}{\partial C}\right)^2 u_C^2 \tag{3}$$

where u_B and u_C are the uncertainties of B and C, respectively. The derivatives are obtained by differentiation of the virial equation:

$$\frac{\partial V}{\partial B} = \left(\frac{PV}{RT} + \frac{B}{V} + \frac{2C}{V^2}\right)^{-1} = 1.16 \tag{4}$$

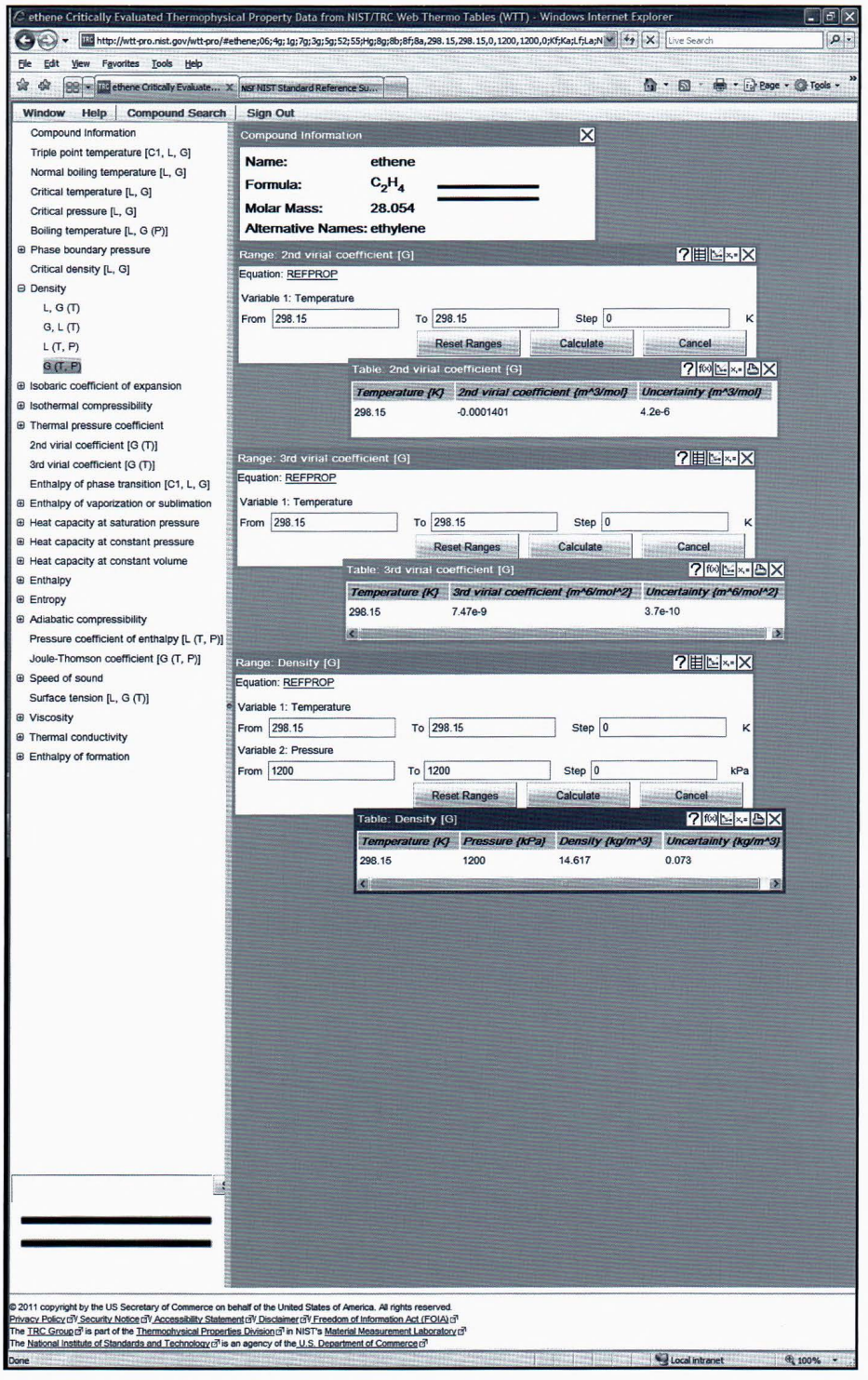
$$\frac{\partial V}{\partial C}=\left(\frac{PV^2}{RT}+B+\frac{2C}{V}\right)^{-1}=6.06\times10^{2}\,\text{mol}\cdot\text{m}^{-3} \qquad (5)$$

Then, the evaluation of the combined expanded uncertainty yields the answer;

$V = (1.9192 \pm 0.0049) \times 10^{-3}\ m^3 \cdot mol^{-1}$.

(b) The critically evaluated density in the gas state is retrieved from WTT at the given temperature and pressure (see Figure 3), $\rho = (14.617 \pm 0.073)\ kg \cdot m^{-3}$. The density is converted to molar volume with the molecular weight of ethane, $W = 28.054\ g \cdot mol^{-1} = 28.054 \times 10^{-3}\ kg \cdot mol^{-1}$ (see Figure 3), $V = W/\rho = 1.91923 \times 10^{-3}\ m^3 \cdot mol^{-1}$. The uncertainty is given by

$$u_v=\left|\frac{\partial V}{\partial \rho}\right|u_\rho=\frac{W}{\rho^2}u_\rho=9.6\times10^{-6}\,\text{m}^3\cdot\text{mol}^{-1} \qquad (6)$$



Then, the calculated molar volume, with uncertainty, is $V = (1.9192 \pm 0.0096) \times 10^{-3}\ m^3 \cdot mol^{-1}$.

As seen, the values obtained in (a) and (b) agree. Identical results reflect the fact that the WTT technology enforces consistency across reported thermodynamic properties.

APPENDIX 2: EXAMPLE FOR A FLUID MECHANICS COURSE

Problem:

2,6-Dimethyl-4-heptanol at 20°C is pumped through a commercial steel pipe at a velocity $u = 1.5\ m \cdot s^{-1}$. The pressure drop per length is recommended, generally, to be $350\ Pa \cdot m^{-1}$. Determine the diameter of the pipe under the given conditions. The surface roughness ε for commercial steel is considered to be 0.05 mm. Accept the following assumptions:

- *2,6-dimethyl-4-heptanol is an incompressible Newtonian fluid.*
- *The pipe is a long horizontal pipe of constant cross section.*
- *No shaft work is done.*
- *Losses in fittings and valves are negligible.*
- *Uncertainties associated with the given conditions are negligible.*

Solution:

The thermophysical properties of saturated 2,6-dimethyl-4-heptanol ex-

Figure 3 (left). *Second and third virial coefficients as a function of temperature and density as a function of temperature and pressure for the gas phase for ethene extracted from WTT for solving the problem described in Appendix 1.*

tracted from WTT at T = 293.15 K (Figure 4) are: density ϱ = (809.75 ± 0.54) kg·m^{-3}; viscosity η = (0.0133 ± 0.0026) Pa·s.

With the assumptions given, the pressure drop is related only to the friction factor. The Fanning friction factor f is defined by:

$$f = \frac{|\Delta p|}{2\rho u^2}\frac{D}{L}, \tag{7}$$

where Δp is the pressure drop, D is the diameter of the pipe, L is the length of the pipe, ρ is the density of the fluid, and u is the flow velocity. The fluid is assumed to have a turbulent flow, and the Colebrook equation is used to calculate the Fanning friction factor for turbulent flow:

$$\frac{1}{\sqrt{f}} = -4\log_{10}\left(\frac{\varepsilon/D}{3.7} + \frac{1.256}{Re\sqrt{f}}\right), \tag{8}$$

where Re is the Reynolds number,

$$Re \equiv \frac{Du\rho}{\eta} \tag{9}$$

Substitution of the expressions for Re and f into the Colebrook equation results in a non-linear equation with respect to D. Its numerical solution yields D = 8.744 × 10^{-2} m. The earlier assumption of turbulent flow is verified by evaluation of the Reynolds number by use of the value of D, which yields Re = 7.985 × 10^4. The combined expanded uncertainty of the diameter is expressed by,

$$u_D^2 = \left(\frac{\partial D}{\partial \rho}\right)^2 u_\rho^2 + \left(\frac{\partial D}{\partial \eta}\right)^2 u_\eta^2 \tag{10}$$

The derivatives in the above quotation are evaluated numerically by use of the central difference approximation,

$$\frac{\partial D}{\partial x} \approx \frac{D(x+\Delta x) - D(x-\Delta x)}{2\Delta x}, \tag{11}$$

where x is the independent variable (either ρ or η), and Δx is its increment. The convergence of the central difference approximation was tested with increments of 1 % and 0.1 % of the initial value for each variable. The converged results are

$$\frac{\partial D}{\partial \rho} = 6.30\times10^{-5}\,m^4\cdot kg^{-1}, \tag{12}$$

$$\frac{\partial D}{\partial \eta} = 1.31\,m^2\cdot s\cdot kg^{-1} \tag{13}$$

The combined expanded uncertainty for D is equal to:

$$u_D = 3.4\times10^{-3}\,m \tag{14}$$

Finally,

$$D = (8.74\pm0.34)\times10^{-2}\,m \tag{15}$$

The combined expanded uncertainty in this example is dominated by the uncertainty of viscosity, as the density value is much more accurate (0.1 % uncertainty vs. 20 % uncertainty). Indeed, $(\partial D/\partial \rho)u_\rho$ equals 0.000034 m and $(\partial D/\partial \eta)u_\eta$ equals 0.0034 m.

APPENDIX 3: EXAMPLE FOR A HEAT AND MASS TRANSFER COURSE

Problem:

A counter-flow, concentric-tube heat exchanger is used to cool 2-aminoethanol for capturing carbon dioxide. The flow rate of cooling methyloxirane through the inner tube (D_i = 25 mm) is $\dot{m}_c$ = 0.2 kg·s^{-1}, while the flow rate of 2-aminoethanol through the outer annulus (D_o = 45 mm) is $\dot{m}_h$ = 0.1 kg·s^{-1}. The 2-aminoethanol and methyloxirane enter at a temperature of 100 °C and 30°C, respectively. How long must the tube be made if the outlet temperature of the 2-aminoethanol is to be 60°C? Accept the following assumptions:

- *Negligible heat loss to the surroundings*
- *Negligible kinetic and potential energy changes*
- *Negligible tube wall thermal resistance and fouling factors*
- *Temperature and flow rate have negligible uncertainties*
- *Heat capacities of both components at constant pressure are equal to those at the saturation line.*
- *Temperature, viscosity, and thermal conductivity of both streams are equal to those at the saturation line.*

Also use information provided in Table 1 to interpolate the necessary Nusselt number as a function of (D_i/D_o). The Nusselt number is assumed also to have negligible uncertainty.

Solution:

To calculate properties, the average temperature of the methyloxirane and 2-aminoethanol streams must be determined. For the 2-aminoethanol stream, this temperature is $\bar{T}_h$

TABLE 1
Nusselt number for fully developed laminar flow in a circular tube annulus with one surface insulated and the other at constant temperature.*†

D_i/D_o	Nu_i	Nu_o
0	-	3.66
0.05	17.46	4.06
0.10	11.56	4.11
0.25	7.37	4.23
0.50	5.74	4.43
≈1.00	4.86	4.86

* Kays, W.M., and H.C. Perkins, in: Rohsenow, W.M., and J.P. Hartnett, eds., *Handbook of Heat Transfer*, Chapter 7. New York: McGraw-Hill (1972)

† D_i and D_o are the diameters of inner tube and outer annulus, respectively. Nu_i and Nu_o are the Nusselt numbers of inner and outer surfaces, respectively.

= 353.15 K. For the methyloxirane stream, this temperature $\bar{T}_c$ can be found only by simultaneous determination of the final temperature of the methyloxirane $T_{c,o}$ and the heat capacity of the methyloxirane stream at its average temperature $C_{s,c}$. We assume $\bar{T}_c$ to be 43.6 °C = 316.75 K as an initial approximation. The saturated properties of methyloxirane at $\bar{T}_c$ = 316.75 K extracted from WTT (Figure 5) are: heat capacity C_s = (126.4 ± 1.8) J·mol^{-1}·K^{-1}; viscosity η = (2.50 ± 0.19) × 10^{-4} Pa·s; thermal conductivity, k = (0.115 ± 0.013) W·m^{-1}·K^{-1}. For 2-aminoethanol at $\bar{T}_h$ = 353.15 K, these properties are (Figure 5): C_s = (181.0 ± 2.6) J·mol^{-1}·K^{-1}; viscosity η = (2.996 ± 0.073) × 10^{-3} Pa·s; thermal conductivity, k = (0.234 ± 0.005) W·m^{-1}·K^{-1}. The molecular masses of methyloxirane and 2-aminoethanol are W_c = 0.05808 kg·mol^{-1} and W_h = 0.06108 kg·mol^{-1}, respectively.

The required heat transfer rate q may be obtained from the overall balance for the hot fluid, 2-aminoethanol:

$$q = \dot{m}_h \frac{C_{s,h}}{W_h}\left(T_{h,i} - T_{h,o}\right) = 11.85\,\text{kW} \qquad (16)$$

where $\dot{m}_h$ is the flow rate of the hot stream (2-aminoethanol). $T_{h,i}$ and $T_{h,o}$ are the inlet and outlet temperature of the hot stream, respectively.

The methyloxirane outlet temperature is obtained from the corresponding balance,

$$q = \dot{m}_c \frac{C_{s,c}}{W_c}\left(T_{c,o} - T_{c,i}\right), \qquad (17)$$

$$T_{c,o} = \frac{qW_c}{\dot{m}_c C_{s,c}} + T_{c,i} = 330.38\,\text{K} \qquad (18)$$

Then $\bar{T}_c = (330.38 + 303.15)/2 = 316.76$ K, which is close to the initial approximation. Generally, the simultaneous determination of the final temperature of the methyloxirane $T_{c,o}$ and heat capacity of the methyloxirane stream at its average temperature $C_{s,c}$ can be obtained with an iterative process. The required heat exchanger length L may now be obtained from the equation:

$$q = UA\Delta T_{lm}, \qquad (19)$$

where U is the overall convection coefficient, A = $\pi D_i L$ and ΔT_{lm} the log mean temperature difference defined by:

$$\Delta T_{lm} = \frac{\Delta T_2 - \Delta T_1}{\ln\left[\Delta T_2 / \Delta T_1\right]} \qquad (20)$$

$$\Delta T_{lm} = \frac{\left(T_{h,i} - T_{c,o}\right) - \left(T_{h,o} - T_{c,i}\right)}{\ln\left[\left(T_{h,1} - T_{c,o}\right)/\left(T_{h,o} - T_{c,i}\right)\right]} = 36.01\,\text{K} \qquad (21)$$

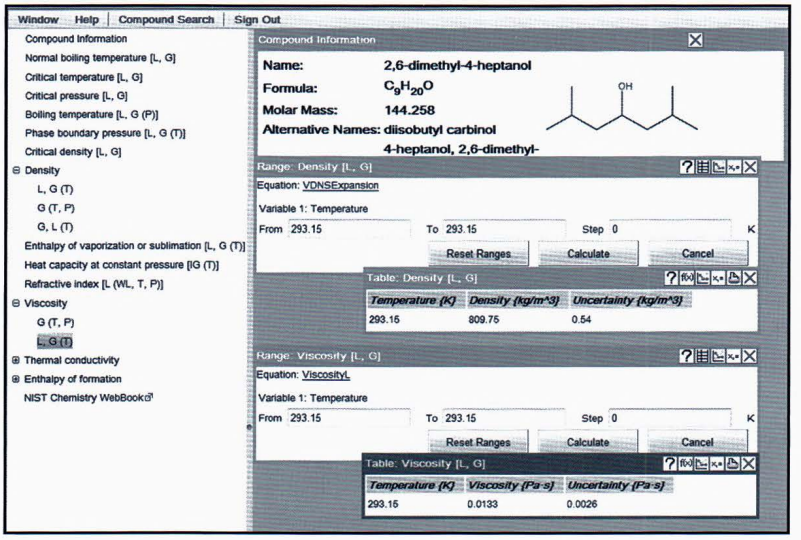


Figure 4. *Density and viscosity for the saturated liquid phase as a function of temperature for 2,6-dimethyl-4- heptanol extracted from WTT for solving the problem described in Appendix 2.*

For methyloxirane flow through the tube, the Reynolds number Re is

$$\text{Re} = \frac{\rho u D_i}{\eta} = \frac{\rho D_i}{\eta} \times \frac{\dot{m}_c}{\rho \pi D_i^2 / 4} = \frac{4\dot{m}_c}{\pi D_i \eta} = 40744 \qquad (22)$$

Accordingly, the flow is turbulent and the Nusselt number can be computed from the scaling equation

$$\text{Nu} = 0.023\,\text{Re}^{4/5}\,\text{Pr}^{0.4}, \qquad (23)$$

where the Prandtl number Pr = $C_s\eta/W_c k$. Substitution of properties for methyloxirane yields Pr = 4.731 and Nu = 208.81. The resulting convection coefficient is

$$h_i = \text{Nu}\frac{k}{D_i} = 960.5\,\text{W}\cdot\text{m}^{-2}\cdot\text{K}^{-1} \qquad (24)$$

For the flow of 2-aminoethanol through the annulus, the hydraulic diameter D_h is

$$D_h = D_c - D_i = 0.02\,\text{m}, \qquad (25)$$

and the Reynolds number is

$$\text{Re} = \frac{\rho u D_h}{\eta} = \frac{\rho D_h}{\eta} \times \frac{\dot{m}_h}{\rho\pi\left(D_o^2 - D_i^2\right)/4} = \frac{4\dot{m}_h}{\pi\left(D_o + D_i\right)\eta} = 607.1 \qquad (26)$$

The annular flow, therefore, is laminar.

Linear interpolation between the values provided in Table1 for the given (D_i/D_o) results in Nu_i =5.64.

The convection coefficient for the outer flow is

$$h_o = \text{NU}_i\frac{k}{D_h} = 66.01\,\text{W}\cdot\text{m}^{-2}\cdot\text{K}^{-1} \qquad (27)$$

The overall convection coefficient is, then,

$$U = \frac{1}{(1/h_i)+(1/h_o)} = 61.77\ W \cdot m^{-2} \cdot K^{-1} \qquad (28)$$

and the sought length is

$$L = \frac{q}{U\pi D_i \Delta T_{lm}} = 67.85\,m \qquad (29)$$

Rigorous uncertainty analysis for this example is not feasible due to the number of approximations made in the process (such as constant thermophysical properties taken at a representative temperature value). The following analysis is performed to illustrate the effect of typical experimental uncertainties of the input thermophysical properties on the resulting value in practical calculations. As previously, all partial derivatives were evaluated by use of a central difference approximation with increments of 1 % and 0.1 %. The results are summarized in Table 2. As seen, the uncertainty of the thermal conductivity of 2-aminoethanol has the largest effect on the predicted length of heat exchanger, followed by the uncertainty of heat capacity of 2-aminoethanol. Uncertainties in input thermophysical properties alone produce roughly 2.8 % uncertainty in the length of the heat exchanger. ❐

TABLE 2
Analysis of the impact of the uncertainties in thermophysical properties of methyloxirane and 2-aminoethanol on the length of the heat exchanger of a pipe-inside-pipe type.*

x	$\frac{\partial L}{\partial x}$	$\left\|\frac{\partial L}{\partial x}\right\| u_x$
methyloxirane		
C_s	-0.188 m·mol·K·J^{-1}	0.188 m
η	6.98×10^3 m·Pa^{-1}·s^{-1}	0.133 m
k	-22.8 m^2·K·W^{-1}	0.296 m
2-aminoethanol		
C_s	0.501 m·mol·K·J^{-1}	1.30 m
η	0 m·Pa^{-1}·s^{-1}	0 m
k	-271 m^2·K·W^{-1}	1.36 m

* x, a property (C_s, η, or k); C_s, heat capacity in the liquid phase at the saturation line; η, viscosity in the liquid phase; k,thermal conductivity in the liquid phase; L the length of the heat exchanger;

$\left\|\frac{\partial L}{\partial x}\right\| u_x$, uncertainty of the required length of the heat exchanger associated with the uncertainty of the property x. For 2-aminoethanol,$\partial L/\partial\eta$ is zero because the flow is laminar.

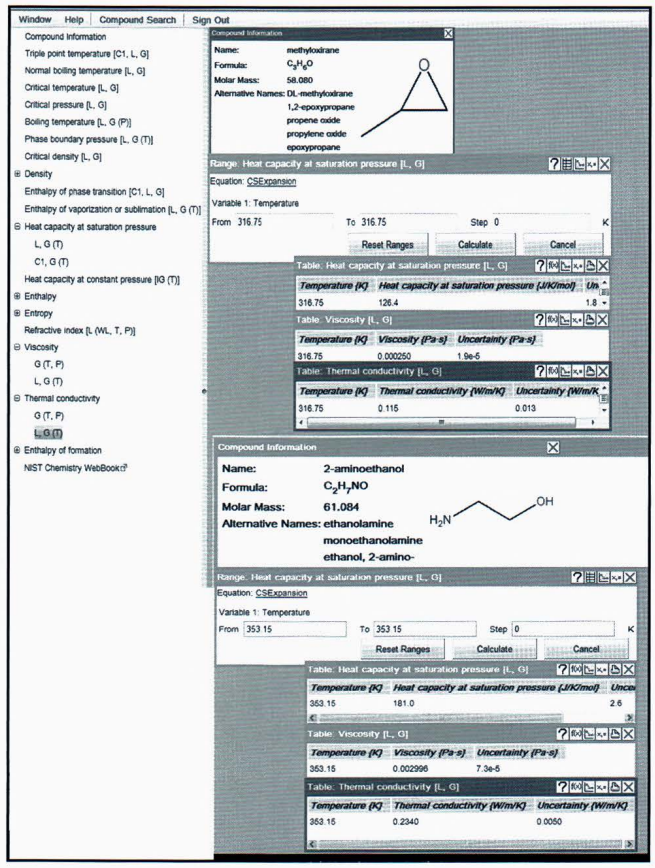


Figure 5. *Heat capacity, viscosity, and thermal conductivity for the liquid phase at saturation pressure for methyloxirane and 2-aminoethanol as a function of temperature extracted from WTT for solving the problem described in Appendix 3.*