Fortschritt-Berichte VDI

VDI

Reihe 6

Energietechnik

Dipl.-Ing. (FH) Matthias Kunick,
Görlitz

Nr. 618

Fast Calculation of Thermophysical Properties in Extensive Process Simulations with the Spline-Based Table Look-Up Method (SBTL)

Fast Calculation of Thermophysical Properties in Extensive Process Simulations with the Spline-Based Table Look-Up Method (SBTL)

Submitted to the
Faculty of Mechanical Science and Engineering of the
Technische Universität Dresden
in partial fulfillment of the requirements for the degree of
Doktor-Ingenieur (Dr.-Ing.)

Dipl.-Ing. (FH) Matthias Kunick
born December 26, 1978 in Altdöbern, Germany

Day of submittal: June 9, 2017
Day of defense: October 23, 2017

Fortschritt-Berichte VDI

Reihe 6

Energietechnik

Dipl.-Ing. (FH) Matthias Kunick,
Görlitz

Nr. 618

Fast Calculation of Thermophysical Properties in Extensive Process Simulations with the Spline-Based Table Look-Up Method (SBTL)

VDI verlag

Kunick, Matthias
Fast Calculation of Thermophysical Properties in Extensive Process Simulations with the Spline-Based Table Look-Up Method (SBTL)
Fortschr.-Ber. VDI Reihe 6 Nr. 618. Düsseldorf: VDI Verlag 2018.
172 Seiten, 80 Bilder, 58 Tabellen.
ISBN 978-3-18-361806-4, ISSN 0178-9414
€ 62,00/VDI-Mitgliederpreis € 55,80.

Keywords: Spline-Based Table Look-up Method – Thermophysical Properties – Spline-Interpolation – Table Look-Up Method – Equation of State – Process Simulations – Computational Fluid Dynamics – Heat-Cycle Simulations – Transient Processes

The presented Spline-Based Table Look-Up Method (SBTL) is intended to be used for fast and accurate property calculations in computationally extensive process simulations, such as Computational Fluid Dynamics (CFD), heat-cycle calculations, simulations of non-stationary processes, and real-time process optimizations, where conventional multiparameter equations of state may be unsuitable because of their computing time consumption. Through the use of the SBTL method, the results of existing property formulations are accurately reproduced at high computational speed. SBTL property functions, their first derivatives, and inverse functions are continuous and numerically consistent with each other. The developed algorithms are successfully applied in commercial and non-commercial software products for CFD, heat-cycle calculations, and simulations of non-stationary processes. The International Association for the Properties of Water and Steam has adopted the "Guideline on the Fast Calculation of Steam and Water Properties with the Spline-Based Table Look-Up Method (SBTL)".

Bibliographische Information der Deutschen Bibliothek
Die Deutsche Bibliothek verzeichnet diese Publikation in der Deutschen Nationalbibliographie; detaillierte bibliographische Daten sind im Internet unter www.dnb.de abrufbar.

Bibliographic information published by the Deutsche Bibliothek
(German National Library)
The Deutsche Bibliothek lists this publication in the Deutsche Nationalbibliographie (German National Bibliography); detailed bibliographic data is available via Internet at www.dnb.de.

Dissertation

Technische Universität Dresden / Fakultät Maschinenwesen

Datum der Verteidigung: 23. Oktober 2017

Als Manuskript gedruckt. Printed in Germany.
ISSN 0178-9414
ISBN 978-3-18-361806-4

Acknowledgements

This work was carried out within the scope of a co-operative doctoral procedure between the Faculty of Mechanical Science and Engineering at the Technische Universität Dresden and the Faculty of Mechanical Engineering at the Zittau/Görlitz University of Applied Sciences under the supervision of Prof. Dr.-Ing. Uwe Gampe and Prof. Dr.-Ing. Hans-Joachim Kretzschmar. In this acknowledgement, I want to thank all the people who have, in various ways, supported me and my work over the past several years.

I am particularly grateful to Prof. Dr.-Ing. Hans-Joachim Kretzschmar for encouraging me in this work and for his supervision. His ongoing support was crucial for the completion of this work and its success. I am indebted to Prof. Dr.-Ing. Uwe Gampe for enabling the realization of this work and his active interest in it. I am very grateful to Prof. Dr.-Ing. Wolfgang Wagner for his willingness to be a co-referee and for the interesting conversations we had on various occasions.

Furthermore, I am grateful to the members of the International Association for the Properties of Water and Steam (IAPWS), in particular to the members of the IAPWS Task Group "CFD Steam Property Formulation" and to Dr. Allan H. Harvey, Dr. Daniel G. Friend, Dr. Tobias Löw, Dr. Reiner Pawellek, and Ingo Weber for the fruitful collaboration. I thank Prof. Dr. Francesca di Mare and Pascal Post for the pleasant and productive collaboration. The opportunity to test the property functions developed in this work in an advanced Computational Fluid Dynamics code has been of extraordinary importance.

For numerous good reasons, I am extremely grateful to Dr. Eric W. Lemmon. His invitation brought me to the National Institute of Standards and Technology in Boulder (CO/USA) where he taught me many important lessons on equations of state.

I want to thank my friends and colleagues, in particular but not exclusively, Mareike Weidner, Jutta Pfitzner, Bert Salomo, Christoph Ebermann, Dr.-Ing. Sebastian Herrmann, Roman Schneider, and Felix Rothe from the Faculty of Mechanical Engineering at the Zittau/Görlitz University of Applied Sciences for providing a good working atmosphere. I am also grateful to Prof. Dr.-Ing. Roland Span, Dr.-Ing. Monika Thol ("Alles wird gut!"), Prof. Dr.-Ing. Markus Richter, Dr.-Ing. Andreas Jäger, Dr.-Ing. Robin Wegge, Theresa Eckermann, Stefan Herrig, Sebastian Hielscher, Nico Schneider, and many other present and former staff members of the Chair of Thermodynamics at the Ruhr-Universität Bochum for their friendship and support.

My warmest thanks go to my family, in particular to my wife Kerstin. Their understanding and support rendered this work possible.

Finally, I thank Dr. Eric W. Lemmon, Dr. Ian Bell, JinHyuk Hong, and Jeremy Cope for proofreading this thesis and for their numerous changes to the use of the English language and recommendations for improving this thesis.

The financial support from the Saxon State Ministry for Science and Art is gratefully acknowledged.

Görlitz, October 2017

Contents

List of Symbols and Nomenclature

Symbols	
a	Spline polynomial coefficient
c_p	Specific isobaric heat capacity
c_v	Specific isochoric heat capacity
CTR	Computing-Time Ratio
f	Specific Helmholtz free energy
f	Function
floor()	Round down to nearest integer
$\boldsymbol{F}$	Vector of functions
g	Specific Gibbs free energy
h	Specific enthalpy
i	Interval index in x_1 direction
(i)	Left node of the interval $\{i\}$ (for knots equal to the nodes)
(i)	Node within the interval $\{i\}$ (for knots between the nodes)
$\{i\}$	Interval $\overline{x}_{1,i} \le \overline{x}_1 < \overline{x}_{1,i+1}$ (for knots equal to the nodes)
$\{i\}$	Interval $\overline{x}^{\mathrm{K}}_{1,i} \le \overline{x}_1 < \overline{x}^{\mathrm{K}}_{1,i+1}$ (for knots between the nodes)
(i,j)	Lower left node of the cell $\{i,j\}$ (for knots equal to the nodes)
(i,j)	Node within the cell $\{i,j\}$ (for knots between the nodes)
$\{i,j\}$	Cell defined by the intervals $\{i\}$ and $\{j\}$
I	Number of nodes along x_1
j	Interval index in x_2 direction
$\{j\}$	Interval $\overline{x}_{2,j} \le \overline{x}_2 < \overline{x}_{2,j+1}$ (for knots equal to the nodes)
$\{j\}$	Interval $\overline{x}^{\mathrm{K}}_{2,j} \le \overline{x}_2 < \overline{x}^{\mathrm{K}}_{2,j+1}$ (for knots between the nodes)
J	Number of nodes along x_2
$\boldsymbol{J}$	Jacobian matrix
p	Pressure
R	Specific gas constant
s	Specific entropy
T	Absolute temperature
TOL	Tolerance for iterative procedures (typically less than or equal to 10^{-8})
u	Specific internal energy
v	Specific volume
w	Speed of sound
x	Vapor fraction
x_1	Independent variable
$\overline{x}_1$	Transformed independent variable
x_2	Independent variable
$\overline{x}_2$	Transformed independent variable

X	Vector of unknowns
z	Dependent variable
$\overline{z}$	Transformed dependent variable

Greek Symbols

δ	Reduced density
Φ	Reduced Helmholtz free energy
γ	Reduced Gibbs free energy
η	Reduced enthalpy
η	Dynamic viscosity
θ	Reduced temperature
λ	Thermal conductivity
π	Reduced pressure
ρ	Mass density
τ	Inverse reduced temperature

Subscripts

B	At region boundary
c	At the critical point
i	Interval index in x_1 direction
j	Interval index in x_2 direction
liq_spin	At liquid spinodal
min	Minimum value
max	Maximum value
perm	Permissible value
RMS	Root-mean-square value of a quantity, see below
s	At saturation
0	Reference state
*	Reducing quantity

Superscripts

AUX	Auxiliary spline function
G	Spline function for the gas region
HT	Spline function for the high-temperature region
INV	Inverse spline function
K	Knot
L	Spline function for the liquid region
MG	Spline function for the metastable-vapor and the gas region
SPL	Spline function

T	Transposed
-T	Inverted and transposed
o	Ideal-gas state; ideal-gas part
r	Residual part
′	State of saturated liquid
″	State of saturated vapor

The root-mean-square value is

$$\Delta x_{\mathrm{RMS}} = \sqrt{\frac{1}{N}\sum_{n=1}^{N}(\Delta x_n)^2}\ ,$$

where Δx_n can be either the absolute or percentage difference between the corresponding quantities x; N is the number of Δx_n values (depending on the property, between 10 million and 100 million points are uniformly distributed over the respective range of validity).

Definitions	
Backward function	Inverse function for $x_1(z)$, $x_1(z,x_2)$, or $x_2(x_1,z)$
Forward function	Explicit function for $z(x_1)$ or $z(x_1,x_2)$
Knot	Connection point of neighboring spline polynomials
Node	Point to be intersected by a spline polynomial
Spline function	Continuous, piecewise-defined function consisting of several spline polynomials
Spline polynomial	Polynomial whose coefficients are determined with a spline algorithm

Abstract

Numerical process simulations, such as flow analysis with Computational Fluid Dynamics (CFD), power-plant design with heat cycle calculations, and real-time process optimizations, are widely used in power engineering. These simulations are computationally expensive, especially when transient processes are considered. During the computation, the thermo-physical properties of the utilized working fluids need to be calculated extremely often. Therefore, fast and accurate property functions are required. Furthermore, numerical process simulations require these property functions to be continuously differentiable once and numerically consistent with each other. Because of their computing-time consumption, accurate multiparameter equations of state are unsuitable for some extensive process simulations and faster, but often less accurate, property calculation algorithms are applied.

In order to provide fast and accurate property calculation algorithms for computationally expensive process simulations, the International Association for the Properties of Water and Steam (IAPWS) has established the task group "CFD Steam Property Formulation". Within this task group, the Spline-Based Table Look-up Method (SBTL) has been developed in this work. The SBTL method combines polynomial spline interpolation techniques and specialized coordinate transformations to reproduce the results of an underlying property formulation, *e.g.*, the industrial formulation IAPWS-IF97 or the scientific formulation IAPWS-95 for water and steam, with high accuracy and low computing time. Depending on the order of the applied spline polynomials, SBTL property functions are at least one time continuously differentiable. Furthermore, the so-called inverse spline functions are numerically consistent with their corresponding forward spline functions, *e.g.*, $u(p,v)$ and $p(v,u)$.

In this work, the development of the SBTL method, as well as its practical application for property calculations in numerical process simulations, is described. To begin, currently applied property calculation methods are discussed regarding their accuracy and their computing-time consumption. From the obtained findings, conclusions for the development of a new property calculation method are drawn. Then the developed SBTL method is described in detail. The SBTL method is exemplified by its application to the industrial formulation IAPWS-IF97 and the scientific formulation IAPWS-95 along with the current transport property formulations for water and steam. For these formulations, SBTL property functions of specific volume and specific internal energy (v,u), as required in CFD, are presented. From these SBTL property functions, numerically consistent inverse functions for calculations from (p,v) and (u,s) are derived. Analogously, SBTL property functions of pressure and specific enthalpy (p,h), as required in heat cycle calculations, are described. With these functions thermodynamic and transport properties, their derivatives, and inverse functions are calculable in the single-phase, two-phase, and metastable regions. The properties calculated from the SBTL property functions represent those of the underlying IAPWS standards with very high accuracy. Typically, the maximum relative deviations amount to between 1 to 100 ppm depending on the property and the range of state. Computations from the (v,u) spline functions are more than 100 times faster than calculations with IAPWS-IF97 and are more than 200 times faster than calculations with IAPWS-95.

The applicability of the SBTL method is verified in the CFD code TRACE, developed at the German Aerospace Center (DLR), as well as in two different heat cycle calculation software

tools, namely in KRAWAL-modular, developed by SIEMENS PG, and in EBSILON® Professional, developed by STEAG Energy Services. Additionally, the use of the SBTL method is verified in RELAP-7, the thermalhydraulic program for the simulation of transient processes in nuclear reactors and plants, developed by the Idaho National Laboratory (INL). The numerical results of the process simulations with the SBTL method show negligible differences from those obtained through the direct application of the underlying property formulations, but the overall computing times are reduced significantly.

In order to apply the SBTL method to property functions for any fluid, the software FluidSplines has been developed.

Based on the results outlined above, the "IAPWS Guideline on the Fast Calculation of Steam and Water Properties with the Spline-Based Table Look-Up Method (SBTL)" has been developed, which was adopted by IAPWS in 2015.

Kurzfassung

Numerische Prozesssimulationen, wie beispielsweise rechnergestützte Analysen strömungsmechanischer Vorgänge (englisch: Computational Fluid Dynamics, CFD), Kreisprozessberechnungen zur Auslegung kraftwerkstechnischer Anlagen und Betriebsoptimierungen in Echtzeit, werden in der Energietechnik vielfältig eingesetzt. Diese Simulationen sind rechentechnisch sehr aufwändig, insbesondere wenn instationäre Vorgänge betrachtet werden müssen. Während der Prozessberechnung müssen die thermophysikalischen Eigenschaften der verwendeten Arbeitsfluide extrem häufig ermittelt werden. Hierfür werden schnelle und genaue Stoffwertfunktionen benötigt. Die verwendeten Stoffwert-Berechnungsalgorithmen müssen einmal stetig differenzierbar und numerisch konsistent zueinander sein. Aufgrund ihrer langen Rechenzeiten sind genaue empirische Zustandsgleichungen für den Einsatz in aufwändigen numerischen Prozesssimulationen nicht geeignet, weshalb auf einfachere, jedoch häufig auch ungenauere Stoffwert-Berechnungsalgorithmen zurückgegriffen wird.

Um schnelle und gleichzeitig sehr genaue Stoffwert-Berechnungsalgorithmen zur Verfügung zu stellen, hat die International Association for the Properties of Water and Steam (IAPWS) die Task Group “CFD Steam Property Formulation“ gebildet. Innerhalb dieser Task Group wurde das Spline-basierte Table Look-up Verfahren (SBTL) im Rahmen dieser Arbeit entwickelt. Das SBTL Verfahren kombiniert Spline-Interpolationsalgorithmen mit speziellen Koordinatentransformationen um die zugrunde gelegte Stoffwertgleichung, beispielsweise die Industrieformulation IAPWS-IF97 oder die wissenschaftliche Formulation IAPWS-95 für Wasser und Wasserdampf, mit hoher Genauigkeit und geringer Rechenzeit wiederzugeben. Abhängig vom Grad der verwendeten Spline-Polynome sind SBTL Stoffwertfunktionen mindestens einmal stetig differenzierbar. Zudem ermöglicht das SBTL Verfahren die Berechnung numerisch konsistenter Umkehrfunktionen.

In der vorliegenden Arbeit wird die Entwicklung des SBTL Verfahrens sowie dessen praktische Anwendung zur Stoffwertberechnung in numerischen Prozesssimulationen beschrieben. Dazu werden zunächst die derzeit verwendeten Stoffwert-Berechnungsalgorithmen hinsichtlich ihrer Genauigkeit und ihres Rechenzeitbedarfs diskutiert. Ausgehend von den gewonnenen Erkenntnissen werden Zielstellungen und Ansätze für die Entwicklung eines neuen Stoffwert-Berechnungsverfahrens formuliert. Anschließend wird das entwickelte SBTL Verfahren im Detail erläutert. Das SBTL Verfahren wird beispielhaft auf die Industrieformulation IAPWS-IF97, die wissenschaftliche Formulation IAPWS-95 sowie die aktuellen IAPWS Formulationen für die Transporteigenschaften für Wasser und Wasserdampf angewendet. Für diese zugrunde liegenden Gleichungen werden SBTL Stoffwertfunktionen von spezifischem Volumen und spezifischer innerer Energie (v,u), wie sie beispielsweise in CFD Simulationen zum Einsatz kommen, vorgestellt. Zudem werden aus diesen SBTL Stoffwertfunktionen numerisch konsistente Umkehrfunktionen von (p,v) und (u,s) entwickelt. Analog werden SBTL Stoffwertfunktionen für die in Kreisprozessberechnungen häufig auftretende Variablenkombination von Druck und spezifischer Enthalpie (p,h) sowie entsprechende Umkehrfunktionen von (p,T), (p,s) und (h,s) beschrieben. Mit diesen Funktionen können die thermophysikalischen Eigenschaften sowie deren Ableitungen und Umkehrfunktionen im Ein- und Zweiphasengebiet berechnet werden. Die aus den SBTL Funktionen berechneten Stoffwerte stimmen mit den zugrundeliegenden Gleichungen mit sehr hoher

Genauigkeit überein, beanspruchen aber wesentlich geringere Rechenzeiten. Typische maximale Abweichungen betragen je nach Stoffwertfunktion und Gültigkeitsbereich 1 bis 100 ppm. Im Vergleich mit dem Industriestandard IAPWS-IF97 sind die SBTL Funktionen von (v,u) mehr als 100-mal schneller. Gegenüber dem wissenschaftlichen Standard IAPWS-95 sind diese Funktionen mehr als 200-mal schneller.

Die Anwendbarkeit des SBTL Verfahrens wird im CFD-Code TRACE, entwickelt am Deutschen Zentrum für Luft- und Raumfahrt (DLR), sowie in den Kreisprozessberechnungsprogrammen KRAWAL-modular, entwickelt von SIEMENS PG, und EBSILON® Professional, entwickelt von STEAG Energy Services, nachgewiesen. Weiterhin wird der Nutzen des SBTL Verfahrens in RELAP-7, der vom Idaho National Laboratory (INL) entwickelten Software zur Simulation instationärer Prozesse in Kernreaktoren, aufgezeigt. Die Ergebnisse der Prozessberechnungen mit dem SBTL Verfahren weisen gegenüber der direkten Verwendung der zugrunde liegenden Gleichungen vernachlässigbare Differenzen auf. Die Gesamtrechenzeiten der Prozessberechnungen werden jedoch signifikant reduziert.

Für die Anwendung des SBTL Verfahrens auf weitere Stoffwertfunktionen und beliebige Fluide ist in dieser Arbeit die Software FluidSplines entwickelt worden.

Auf Grundlage der Ergebnisse dieser Arbeit ist die neue “IAPWS Guideline on the Fast Calculation of Steam and Water Properties with the Spline-Based Table Look-Up Method (SBTL)” erarbeitet worden, welche von der IAPWS im Jahr 2015 als internationale Richtlinie verabschiedet wurde.