

Supplementary Backward Equations $v(p, T)$ for the Critical and Supercritical Regions (Region 3) of the Industrial Formulation IAPWS-IF97 for Water and Steam

K. Knobloch, I. Stöcker, H.-J. Kretzschmar
University of Applied Sciences of Zittau and Görlitz, Germany
Department of Technical Thermodynamics

A. Dittmann
Technical University of Dresden, Germany
Department of Thermodynamics

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Numerical Consistency Requirements

Calculation of functions from (p, T) in region 3:

$$f_3^{97}(T, v) \longrightarrow p_3^{97}, h_3^{97}, s_3^{97}, c_{p,3}^{97}, w_3^{97}, \dots = f(T, v)$$

Required functions: $h_3^{97}, s_3^{97}, c_{p,3}^{97}, w_3^{97}, \dots = f(p, T) \longrightarrow$ **Iteration of v for given p and T**

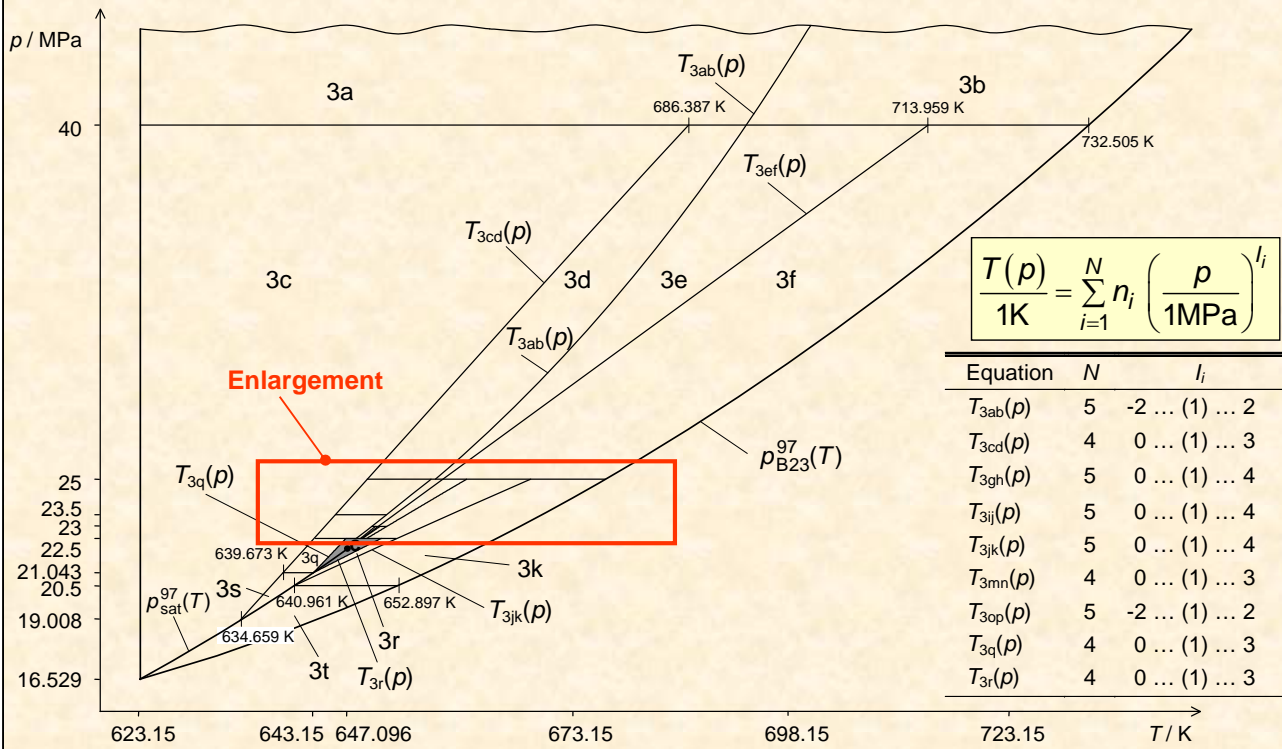
Numerical consistency relation:

$$\begin{array}{c} \boxed{f_3^{97}(T, v)} \longrightarrow \boxed{p_3^{97}(T, v)} \longrightarrow \boxed{v_3(p, T)} \\ \downarrow \\ \boxed{\left| \frac{\Delta v}{v} \right| = \frac{v_3[p_3^{97}(T, v), T] - v}{v} \leq \left| \frac{\Delta v}{v} \right|_{\text{tol}}} \longrightarrow \boxed{\left| \frac{\Delta v}{v} \right|_{\text{tol}} = 0.001\%} \end{array}$$

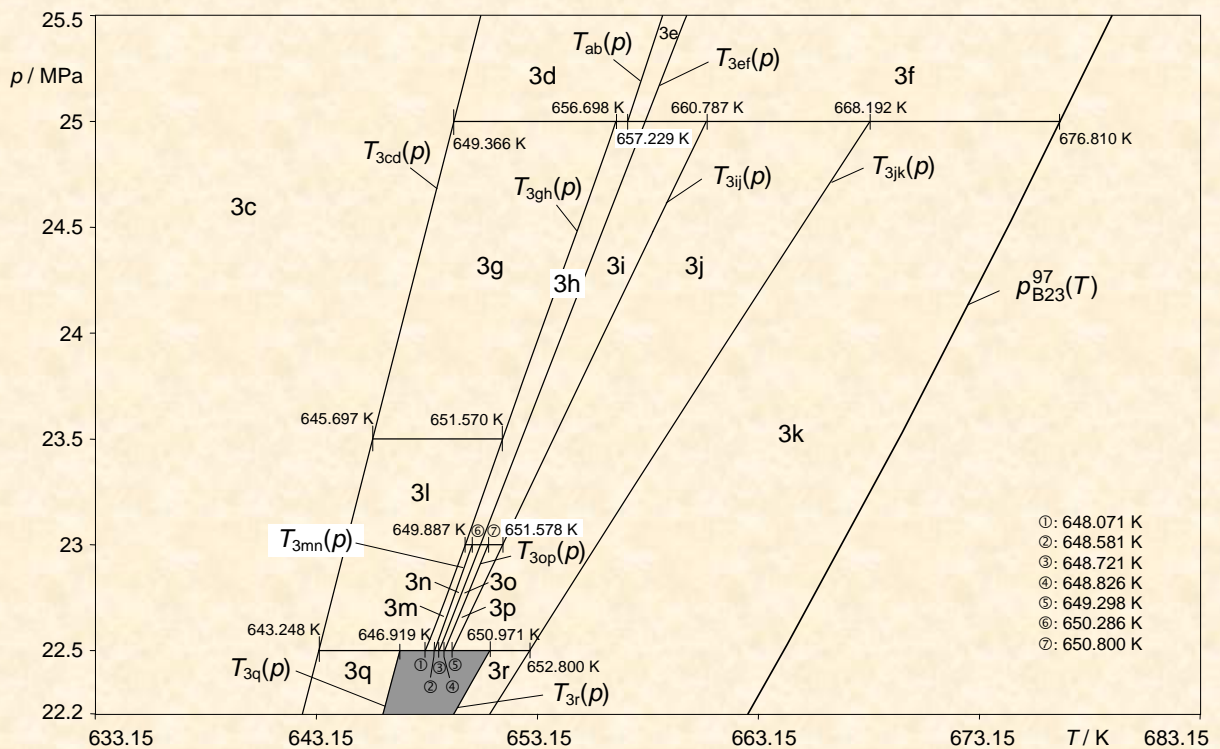
Iteration accuracy in process calculation:

$$\left. \begin{array}{l} \boxed{h_3^{97}(p, T), s_3^{97}(p, T)} \longleftrightarrow \boxed{\left| \frac{\Delta h}{h} \right|, \left| \frac{\Delta s}{s} \right| = 0.001\%} \\ \boxed{c_{p,3}^{97}(p, T), w_3^{97}(p, T)} \longleftrightarrow \boxed{\left| \frac{\Delta c_p}{c_p} \right|, \left| \frac{\Delta w}{w} \right| = 0.01\%} \end{array} \right\} \longleftrightarrow \boxed{\left| \frac{\Delta v}{v} \right| = 0.001\%}$$

Structure of the Equation Set



Structure of the Equation Set



Backward Equations $v(p, T)$ for Region 3

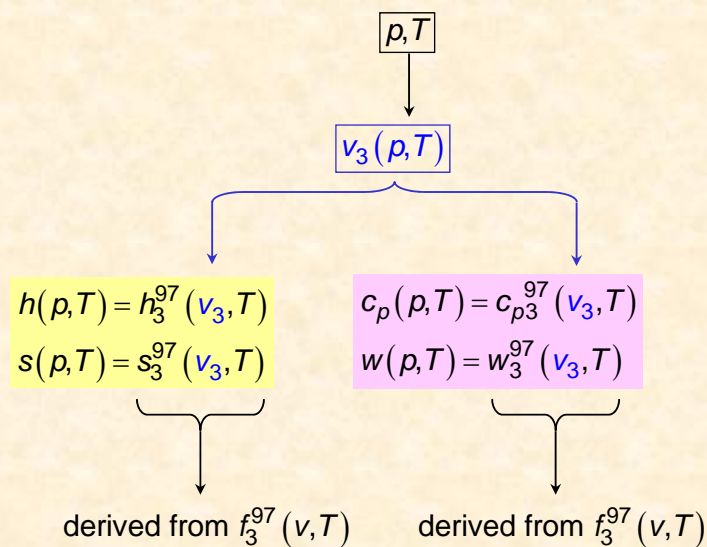
results of the structure optimization

$$\frac{v(p, T)}{v^*} = \left[\sum_{i=1}^N n_i \left[\left(\frac{p}{p^*} - a \right)^c \right]^{l_i} \left[\left(\frac{T}{T^*} - b \right)^d \right]^{j_i} \right]^e$$

determined by optimization

Sub-region	v^* m ³ kg ⁻¹	p^* MPa	T^* K	a	b	c	d	e	N
3a	0.0024	100	760	0.085	0.817	1	1	1	30
3b	0.0041	100	860	0.280	0.779	1	1	1	32
3c	0.0022	40	690	0.259	0.903	1	1	1	35
3d	0.0029	40	690	0.559	0.939	1	1	4	38
3e	0.0032	40	710	0.587	0.918	1	1	1	29
3f	0.0064	40	730	0.587	0.891	0.5	1	4	42
3g	0.0027	25	660	0.872	0.971	1	1	4	38
3h	0.0032	25	660	0.898	0.983	1	1	4	29
3i	0.0041	25	660	0.910	0.984	0.5	1	4	42
3j	0.0054	25	670	0.875	0.964	0.5	1	4	29
3k	0.0077	25	680	0.802	0.935	1	1	1	34
3l	0.0026	24	650	0.908	0.989	1	1	4	43
3m	0.0028	23	650	1.00	0.997	1	1/4	1	40
3n	0.0031	23	650	0.976	0.997	-	-	-	39
3o	0.0034	23	650	0.974	0.996	0.5	1	1	24
3p	0.0041	23	650	0.972	0.997	0.5	1	1	27
3q	0.0022	23	650	0.848	0.983	1	1	4	24
3r	0.0054	23	650	0.874	0.982	1	1	1	27
3s	0.0022	21	640	0.886	0.990	1	1	4	29
3t	0.0088	20	650	0.803	1.02	1	1	1	33

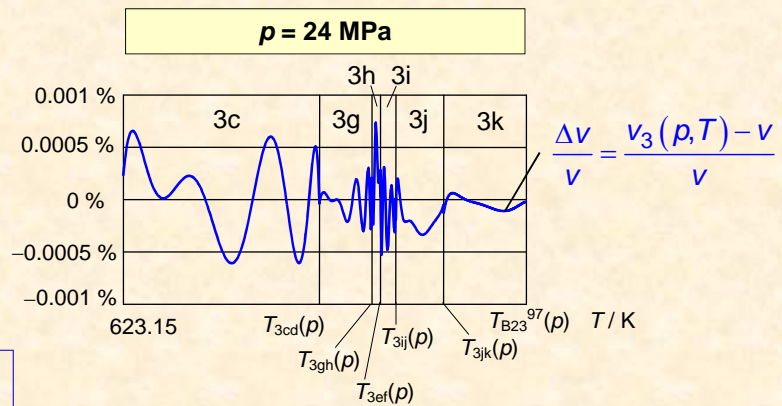
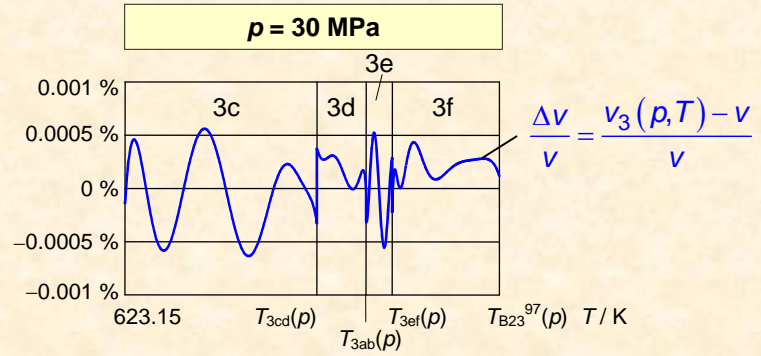
Calculation of Thermodynamic Properties by using the $v_3(p, T)$ Backward Equations



Results for Numerical Consistency with IAPWS-IF97 Basic Equation

Subregion	$ \Delta v/v _{\max}$ %
3a	0.00061
3b	0.00064
3c	0.00080
3d	0.00059
3e	0.00072
3f	0.00068
3g	0.00047
3h	0.00085
3i	0.00067
3j	0.00034
3k	0.00034
3l	0.00033
3m	0.00057
3n	0.00064
3o	0.00031
3p	0.00044
3q	0.00036
3r	0.00037
3s	0.00030
3t	0.00095

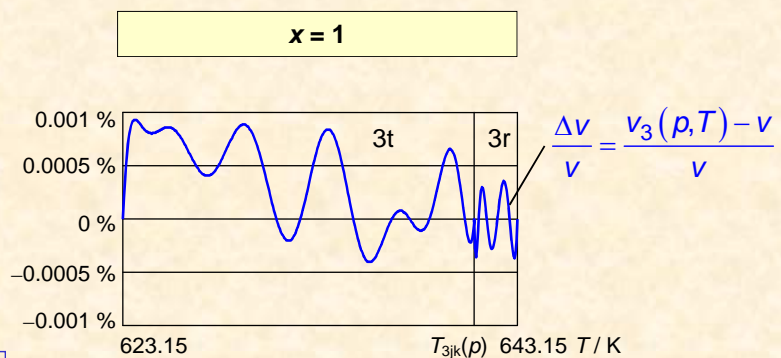
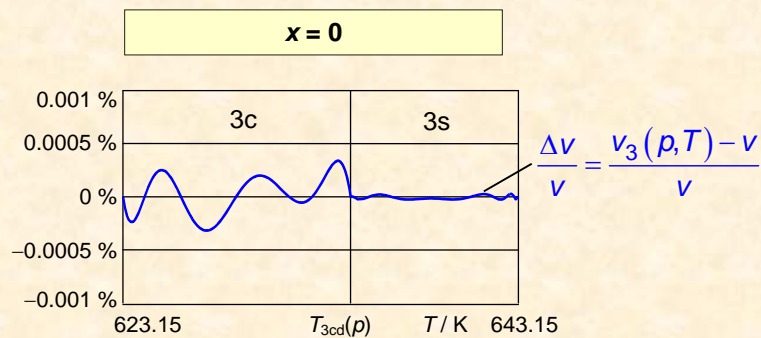
$$|\Delta v/v|_{\max} \leq 0.001\%$$



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$$|\Delta v/v|_{\max} \leq 0.001\%$$



Results for Numerical Consistency with IAPWS-IF97 Basic Equation

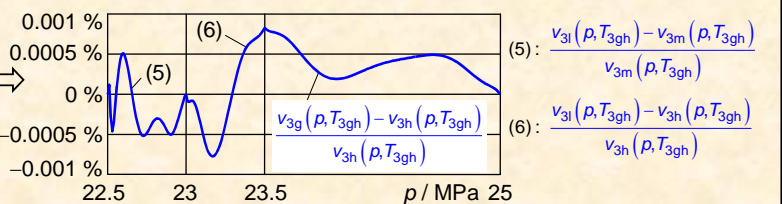
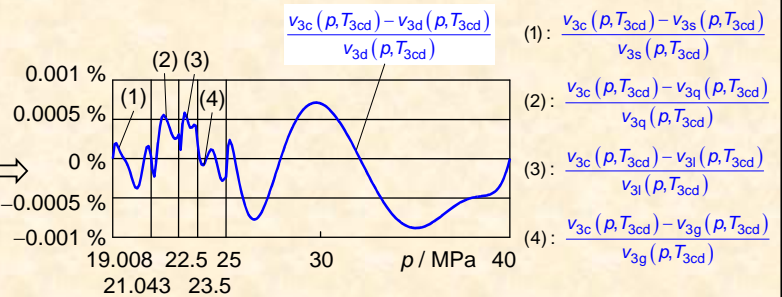
Subregion	$ \Delta h/h _{\max}$ %	$ \Delta s/s _{\max}$ %	$ \Delta c_p/c_p _{\max}$ %	$ \Delta w/w _{\max}$ %
3a	0.00018	0.00026	0.0016	0.0015
3b	0.00018	0.00016	0.0012	0.0008
3c	0.00026	0.00025	0.0059	0.0023
3d	0.00018	0.00014	0.0035	0.0012
3e	0.00018	0.00014	0.0015	0.0006
3f	0.00018	0.00013	0.0015	0.0002
3g	0.00014	0.00011	0.0032	0.0010
3h	0.00023	0.00017	0.0066	0.0006
3i	0.00018	0.00013	0.0019	0.0002
3j	0.00009	0.00007	0.0020	0.0002
3k	0.00008	0.00007	0.0018	0.0002
3l	0.00010	0.00008	0.0035	0.0008
3m	0.00016	0.00011	0.0062	0.0006
3n	0.00017	0.00012	0.0050	0.0002
3o	0.00008	0.00006	0.0007	0.0001
3p	0.00012	0.00009	0.0026	0.0002
3q	0.00012	0.00009	0.0040	0.0010
3r	0.00010	0.00008	0.0030	0.0002
3s	0.00010	0.00007	0.0033	0.0009
3t	0.00022	0.00018	0.0046	0.0004

Maximum Deviations less than: **0.001%**

0.01%

Consistency at Boundary Between Subregions

Subregion Boundary Equation	Between Equations	$ \Delta v/v _{\max}$ %
$T_{3ab}(\rho)$	$v_{3a}(\rho, T), v_{3b}(\rho, T)$	0.00075
	$v_{3d}(\rho, T), v_{3e}(\rho, T)$	0.00061
$T_{3cd}(\rho)$	$v_{3c}(\rho, T), v_{3d}(\rho, T)$	0.00089
	$v_{3c}(\rho, T), v_{3g}(\rho, T)$	0.00029
	$v_{3c}(\rho, T), v_{3i}(\rho, T)$	0.00059
	$v_{3c}(\rho, T), v_{3q}(\rho, T)$	0.00056
	$v_{3c}(\rho, T), v_{3s}(\rho, T)$	0.00039
$T_{3ei}(\rho)$	$v_{3e}(\rho, T), v_{3i}(\rho, T)$	0.00060
	$v_{3h}(\rho, T), v_{3i}(\rho, T)$	0.00061
	$v_{3n}(\rho, T), v_{3o}(\rho, T)$	0.00031
$T_{3gh}(\rho)$	$v_{3g}(\rho, T), v_{3h}(\rho, T)$	0.00083
	$v_{3i}(\rho, T), v_{3h}(\rho, T)$	0.00083
	$v_{3i}(\rho, T), v_{3m}(\rho, T)$	0.00052
$T_{3ij}(\rho)$	$v_{3i}(\rho, T), v_{3j}(\rho, T)$	0.00034
	$v_{3p}(\rho, T), v_{3j}(\rho, T)$	0.00036
$T_{3jk}(\rho)$	$v_{3j}(\rho, T), v_{3k}(\rho, T)$	0.00030
	$v_{3r}(\rho, T), v_{3k}(\rho, T)$	0.00029
$T_{3mn}(\rho)$	$v_{3m}(\rho, T), v_{3n}(\rho, T)$	0.00090
$T_{3op}(\rho)$	$v_{3o}(\rho, T), v_{3p}(\rho, T)$	0.00041



$|\Delta v/v|_{\max} \leq 0.001\%$

Consistency at Boundary Between Subregions

Subregion Boundary Equation	Between Equations	$ \Delta h/h _{\max}$ %	$ \Delta s/s _{\max}$ %	$ \Delta c_p/c_p _{\max}$ %	$ \Delta w/w _{\max}$ %
$T_{3ab}(\rho)$	$v_{3a}(\rho, T), v_{3b}(\rho, T)$	0.00020	0.00020	0.0012	0.0010
	$v_{3d}(\rho, T), v_{3e}(\rho, T)$	0.00017	0.00013	0.0016	0.0006
$T_{3cd}(\rho)$	$v_{3c}(\rho, T), v_{3d}(\rho, T)$	0.00027	0.00021	0.0040	0.0016
	$v_{3c}(\rho, T), v_{3g}(\rho, T)$	0.00009	0.00007	0.0017	0.0007
	$v_{3c}(\rho, T), v_{3i}(\rho, T)$	0.00019	0.00014	0.0039	0.0015
	$v_{3c}(\rho, T), v_{3q}(\rho, T)$	0.00018	0.00014	0.0040	0.0015
	$v_{3c}(\rho, T), v_{3s}(\rho, T)$	0.00012	0.00010	0.0031	0.0011
$T_{3ef}(\rho)$	$v_{3e}(\rho, T), v_{3f}(\rho, T)$	0.00016	0.00012	0.0005	0.0001
	$v_{3h}(\rho, T), v_{3i}(\rho, T)$	0.00016	0.00012	0.0007	0.0001
	$v_{3n}(\rho, T), v_{3o}(\rho, T)$	0.00008	0.00006	0.0004	0.0001
$T_{3gh}(\rho)$	$v_{3g}(\rho, T), v_{3h}(\rho, T)$	0.00022	0.00016	0.0058	0.0006
	$v_{3i}(\rho, T), v_{3h}(\rho, T)$	0.00022	0.00016	0.0064	0.0006
	$v_{3i}(\rho, T), v_{3m}(\rho, T)$	0.00014	0.00011	0.0058	0.0006
$T_{3ij}(\rho)$	$v_{3i}(\rho, T), v_{3j}(\rho, T)$	0.00009	0.00007	0.0010	0.0002
	$v_{3p}(\rho, T), v_{3j}(\rho, T)$	0.00009	0.00007	0.0020	0.0002
$T_{3jk}(\rho)$	$v_{3j}(\rho, T), v_{3k}(\rho, T)$	0.00007	0.00006	0.0008	0.0001
	$v_{3r}(\rho, T), v_{3k}(\rho, T)$	0.00007	0.00006	0.0018	0.0002
$T_{3mn}(\rho)$	$v_{3m}(\rho, T), v_{3n}(\rho, T)$	0.00024	0.00017	0.0070	0.0003
$T_{3op}(\rho)$	$v_{3o}(\rho, T), v_{3p}(\rho, T)$	0.00011	0.00008	0.0013	0.0002

Maximum Deviations less than:

0.001%

0.01%

Consistency at Boundary Between Subregions

Subregion Boundary	Between Equations	$ \Delta v/v _{\max}$ %	$ \Delta h/h _{\max}$ %	$ \Delta s/s _{\max}$ %	$ \Delta c_p/c_p _{\max}$ %	$ \Delta w/w _{\max}$ %
$\rho = 40$ MPa	$v_{3a}(\rho, T), v_{3c}(\rho, T)$	0.00074	0.00022	0.00028	0.0018	0.0019
	$v_{3a}(\rho, T), v_{3d}(\rho, T)$	0.00060	0.00017	0.00013	0.0013	0.0006
	$v_{3b}(\rho, T), v_{3e}(\rho, T)$	0.00062	0.00015	0.00012	0.0009	0.0004
	$v_{3b}(\rho, T), v_{3f}(\rho, T)$	0.00078	0.00018	0.00014	0.0004	0.0002
$\rho = 25$ MPa	$v_{3d}(\rho, T), v_{3g}(\rho, T)$	0.00056	0.00015	0.00011	0.0031	0.0010
	$v_{3d}(\rho, T), v_{3h}(\rho, T)$	0.00056	0.00015	0.00011	0.0021	0.0003
	$v_{3e}(\rho, T), v_{3h}(\rho, T)$	0.00063	0.00017	0.00013	0.0014	0.0002
	$v_{3f}(\rho, T), v_{3i}(\rho, T)$	0.00055	0.00014	0.00011	0.0011	0.0002
	$v_{3f}(\rho, T), v_{3j}(\rho, T)$	0.00060	0.00015	0.00011	0.0015	0.0002
	$v_{3f}(\rho, T), v_{3k}(\rho, T)$	0.00064	0.00013	0.00011	0.0011	0.0002
$\rho = 23.5$ MPa	$v_{3g}(\rho, T), v_{3i}(\rho, T)$	0.00049	0.00015	0.00012	0.0033	0.0011
$\rho = 23$ MPa	$v_{3h}(\rho, T), v_{3m}(\rho, T)$	0.00084	0.00023	0.00017	0.0074	0.0007
	$v_{3h}(\rho, T), v_{3n}(\rho, T)$	0.00085	0.00022	0.00016	0.0047	0.0003
	$v_{3i}(\rho, T), v_{3o}(\rho, T)$	0.00047	0.00012	0.00009	0.0006	0.0002
	$v_{3i}(\rho, T), v_{3p}(\rho, T)$	0.00059	0.00015	0.00012	0.0020	0.0002
$\rho = 22.5$ MPa	$v_{3i}(\rho, T), v_{3q}(\rho, T)$	0.00033	0.00010	0.00008	0.0025	0.0008
	$v_{3j}(\rho, T), v_{3r}(\rho, T)$	0.00035	0.00009	0.00007	0.0015	0.0002
$\rho = \rho_{\text{sat}}$ (643.15 K)	$v_{3q}(\rho, T), v_{3s}(\rho, T)$	0.00033	0.00010	0.00008	0.0036	0.0008
$\rho = 20.5$ MPa	$v_{3k}(\rho, T), v_{3l}(\rho, T)$	0.00042	0.00009	0.00008	0.0019	0.0002

Maximum Deviations less than:

0.001%

0.001%

0.01%

Computing Time in Relation to IAPWS-IF97

Calculation of the function $v(p, T)$:

by iteration from IAPWS-IF97

by new equations

Computing Time
2.5 μ s/call

Computing Time
0.45 μ s/call

CTR
5

$$CTR = \frac{\text{Computing time using IAPWS-IF97 equations only}}{\text{Computing time using the backward equations}}$$

Summary

Backward equations $v(p, T)$ for region 3 of IAPWS-IF97 have been presented.
Functions $h, s, c_p, w(p, T)$ can be calculated using the derivatives of IAPWS-IF97



Numerical consistency is sufficient for process modeling.



Iterations can be avoided.



The calculation of $v(p, T)$ is 5 times faster than IAPWS-IF97.