Eur. Phys. J. Plus (2021) 136:21
https://doi.org/10.1140/epjp/s13360-020-00978-5

THE EUROPEAN PHYSICAL JOURNAL PLUS

Regular Article

Study of specific heat capacities and speed of sound for uranium and uranium fluoride gases

Elif Somuncu[1,a], **Bahtiyar A. Mamedov**[2,b]

[1] Department of Physics, Faculty of Arts and Sciences, Giresun University, Giresun, Turkey
[2] Department of Physics, Faculty of Arts and Sciences, Gaziosmanpaşa University, Tokat, Turkey

Received: 22 September 2020 / Accepted: 29 November 2020

Abstract A new approach is proposed for accurate estimation of thermodynamic properties of nuclear fuels. The method is based on the use of virial coefficients with Lennard-Jones (12-6) potential. The model is applicable to the calculations of thermodynamic quantities of nuclear gases. In this work, we derived new formulae for the calculation of the specific heat capacities and speed of sound of nuclear gases by using the second virial coefficient with Lennard-Jones (12-6) potential. The final results are expressed through the gamma and parabolic cylinder functions that is a better approach to the accurate evaluation of the second virial coefficient. The new approach has been applied to the accurate evaluation of the specific heat capacities and speed of sound for uranium and uranium fluoride gases of U, UF, UF_2, UF_3, UF_4, UF_5 and UF_6 whose importance in nuclear technology is well known. All the results for nuclear gases U, UF,UF_2, UF_3, UF_4, UF_5 and UF_6 are controlled by the calculations in the literature, and their accuracy is confirmed.

1 Introduction

In the theoretical prediction of thermodynamic properties of gases, the virial coefficients play a significant role [1, 2]. In the literature, the definition of the thermodynamic properties of nuclear gases has been the power of the development of the nuclear industry [3–6], and the calculation of the specific heat capacities and speed of sound of nuclear gases has been a strong examination of the correctness of various theories. It is widely known that uranium and uranium fluoride gases constitute the invaluable process of enriching uranium in the field of nuclear industry [6]. The thermodynamic properties such as specific heat capacities and speed of sound are important in the work of various properties of uranium and uranium fluoride gases that are used in the gaseous diffusion, the process of enriching uranium and energy production [7–10]. One of the fundamental problems is to evaluate the thermodynamic properties of gases accurately and precisely. Therefore, the development of new methods to find precise thermodynamic properties of gases still attracts a lot of interest in many groups of researchers. Many equations of state have been suggested for the estimation of thermodynamic properties of gases [11, 12]. One of these equations of state is the virial state

[a] e-mail: elf_smnc@hotmail.com (corresponding author)
[b] e-mail: bamamedov@yahoo.com

equation that is a fundamental equation defining the thermodynamic properties of gases in wide temperature ranges.

The main focus of this article is to investigate the specific heat capacities and speed of sound using the second virial coefficient, consisting of the virial equation of state, at various pressure and temperature and compare the results to the theoretical data available with the literature. Therefore, we proposed analytical expressions which make the fast and accurate evaluation of the specific heat capacities and speed of sound of the gases using the second virial coefficient over Lennard-Jones (12-6) potential. The applications of the obtained analytical formulae of the specific heat capacities and speed of sound to evaluation of gases U, UF, UF_2, UF_3, UF_4, UF_5 and UF_6 show a good rate of convergence and numerical stability. To our knowledge, this study is the first approach to the calculation of thermodynamic properties for uranium and uranium fluoride nuclear materials by using virial coefficients.

2 Definition and expressions of the heat capacities and speed of sound

The heat capacities and speed of sound of gases can be expressed by the second virial coefficient in the forms [13]:

For heat capacity at constant volume

$$C_V - C_V^0 = -\frac{P}{T}\left(2\frac{\mathrm{d}B(T)}{\mathrm{d}T} + \frac{\mathrm{d}^2B(T)}{\mathrm{d}T^2}\right), \tag{1}$$

For heat capacity at constant pressure

$$C_P - C_P^0 = -\left(P\frac{\mathrm{d}^2B(T)}{\mathrm{d}T^2} - \left(\frac{P}{T}\right)^2\left(B(T) - T\frac{\mathrm{d}B(T)}{\mathrm{d}T}\right)^2\right), \tag{2}$$

For speed of sound

$$c_0^2 = \frac{\gamma RT}{M}\left[1 + \frac{P}{RT}\left(2B(T) + 2(\gamma-1)T\frac{\mathrm{d}B(T)}{\mathrm{d}T} + \frac{(\gamma-1)^2}{\gamma}T^2\frac{\mathrm{d}^2B(T)}{\mathrm{d}T^2}\right)\right], \tag{3}$$

In Eqs. (1)–(3), P is the pressure, R is the universal gas constant, T is the temperature, M is the molecular weight, $\gamma = C_P\big/C_V$ is the heat capacity ratio and $B(T)$ is the second virial coefficient. The superscript small zero $\left(^0\right)$ refers to the property of a gas in its ideal state in Eqs. (1)–(3).

It is known that the choice of reliable expressions for the second virial coefficient with Lennard-Jones (12-6) potential is of great significance for accurate and susceptible calculations of the specific heat capacities and speed of sound of gases. Therefore, we use the second virial coefficient in the following form [14]:

$$B\left(T^*\right) = b_0\frac{2}{\sqrt{2}}e^{\frac{1}{2T^*}}\left(\left(\frac{2}{T^*}\right)^{1/4}\Gamma\left(\frac{3}{2}\right)D_{-3/2}\left(-\sqrt{\frac{2}{T^*}}\right) - \left(\frac{2}{T^*}\right)^{3/4}\Gamma\left(\frac{1}{2}\right)D_{-1/2}\left(-\sqrt{\frac{2}{T^*}}\right)\right) \tag{4}$$

here, $b_0 = 2\pi N_A\sigma^3\big/3$, $T^* = k_BT\big/\varepsilon$, the $\Gamma(\alpha)$ is gamma function and $D_\nu(z)$ is parabolic cylinder function.

The analytical formulae for the specific heat capacities and speed of sound are determined by the following form, respectively.

Table 1 The specific heat capacities and speed of sound for U

P (atm)	$T\,(K)$	C_P (kJ/kg K)	C_P (kJ/kg K) [19]	C_V (kJ/kg K)	ΔC_P (kJ/kg K)	ΔC_V (kJ/kg K)	u (m/ s)	u (m/ s) [19]
0.01	800	0.0981192	0.0981	0.0631746	0.00001915	6.53344×10^{-6}	208.381	208.3
	1000	0.101912	0.1019	0.0669734	9.20503×10^{-6}	2.61027×10^{-6}	230.616	230.5
	1500	0.12346	0.1235	0.0885256	2.84005×10^{-6}	5.74706×10^{-7}	270.407	270.3
	2000	0.152668	0.1527	0.117735	1.34033×10^{-6}	2.18962×10^{-7}	301.082	301.0
	2500	0.182015	0.1820	0.147082	7.72855×10^{-7}	1.1059×10^{-7}	328.847	328.7
	3000	0.206336	0.2064	0.171403	5.00303×10^{-7}	6.63532×10^{-8}	355.295	355.2
	3500	0.223448	0.2234	0.188516	3.49131×10^{-7}	4.46603×10^{-8}	380.802	380.7
	4000	0.232847	0.2328	0.197915	2.56799×10^{-7}	3.25847×10^{-8}	405.581	405.4
0.1	800	0.0982916	0.0981	0.0632334	0.0001915	0.0000653344	208.278	208.3
	1000	0.101995	0.1019	0.0669969	0.0000920503	0.0000261027	230.556	230.5
	1500	0.123485	0.1235	0.0885307	0.0000284005	5.74706×10^{-6}	270.383	270.3
	2000	0.15268	0.1527	0.117737	0.0000134033	2.18962×10^{-6}	301.07	301.0
	2500	0.182022	0.1820	0.147083	7.72855×10^{-6}	1.1059×10^{-6}	328.841	328.7
	3000	0.20634	0.2064	0.171404	5.00303×10^{-6}	6.63532×10^{-7}	355.292	355.2
	3500	0.223451	0.2234	0.188516	3.49131×10^{-6}	4.46603×10^{-7}	380.802	380.7
	4000	0.232849	0.2328	0.197915	2.56799×10^{-6}	3.25847×10^{-7}	405.582	405.4
1	800	0.100015	0.0981	0.0638215	0.001915	0.000653344	207.243	208.3
	1000	0.102823	0.1019	0.0672318	0.0009205	0.000261027	229.955	230.5
	1500	0.123741	0.1235	0.0885825	0.000284005	0.0000574706	270.148	270.3
	2000	0.152801	0.1527	0.117757	0.000134033	0.0000218962	300.955	301.0

Table 1 continued

P (atm)	$T\,(K)$	C_P (kJ/kg K)	C_P (kJ/kg K) [19]	C_V (kJ/kg K)	ΔC_P (kJ/kg K)	ΔC_V (kJ/kg K)	u (m/ s)	u (m/ s) [19]
	2500	0.182091	0.1820	0.147093	0.0000772855	0.000011059	328.783	328.7
	3000	0.206385	0.2064	0.17141	0.0000500303	6.63532×10^{-6}	355.267	355.2
	3500	0.223483	0.2234	0.18852	0.0000349131	4.46603×10^{-6}	380.797	380.7
	4000	0.232872	0.2328	0.197918	0.0000256799	3.25847×10^{-6}	405.59	405.4
10	800	0.11725	0.0981	0.0697015	0.01915	0.00653344	196.597	208.3
	1000	0.111108	0.1019	0.0695811	0.00920503	0.00261027	223.859	230.5
	1500	0.126297	0.1235	0.0890997	0.00284005	0.000574706	267.787	270.3
	2000	0.154007	0.1527	0.117954	0.00134033	0.000218962	299.797	301.0
	2500	0.182787	0.1820	0.147193	0.000772855	0.00011059	328.201	328.7
	3000	0.206835	0.2064	0.17147	0.000500303	0.0000663532	355.014	355.2
	3500	0.223797	0.2234	0.18856	0.000349131	0.0000446603	380.747	380.7
	4000	0.233104	0.2328	0.197947	0.000256799	0.0000325847	405.674	405.4

Table 2 The specific heat capacities and speed of sound for UF

P (atm)	$T(K)$	C_P (kJ/kg K)	C_P (kJ/kg K) [19]	C_V (kJ/kg K)	ΔC_P (kJ/kg K)	ΔC_V (kJ/kg K)	u (m/s)	u (m/s) [19]
0.01	800	0.180948	0.1810	0.148597	1.85477×10^{-6}	2.56704×10^{-7}	177.577	177.5
	1000	0.184798	0.1848	0.152448	1.09636×10^{-6}	1.41262×10^{-7}	198.089	198.0
	1500	0.192337	0.1923	0.159987	4.34031×10^{-7}	5.72341×10^{-8}	241.606	241.5
	2000	0.199444	0.1994	0.167094	2.2733×10^{-7}	3.43735×10^{-8}	277.983	277.9
	2500	0.205805	0.2058	0.173455	1.37668×10^{-7}	2.45076×10^{-8}	309.869	309.8
	3000	0.209996	0.2100	0.177647	9.11062×10^{-8}	1.90878×10^{-8}	338.815	338.7
	3500	0.212369	0.2123	0.180019	6.40017×10^{-8}	1.5657×10^{-8}	365.59	365.5
	4000	0.213579	0.2135	0.181229	4.6925×10^{-8}	1.32807×10^{-8}	390.633	390.5
0.1	800	0.180964	0.1810	0.148599	0.0000185477	2.56704×10^{-6}	177.57	177.5
	1000	0.184808	0.1848	0.152449	0.0000109636	1.41262×10^{-6}	198.088	198.0
	1500	0.192341	0.1923	0.159988	4.34031×10^{-6}	5.72341×10^{-7}	241.61	241.5
	2000	0.199446	0.1994	0.167095	2.2733×10^{-6}	3.43735×10^{-7}	277.989	277.9
	2500	0.205806	0.2058	0.173456	1.37668×10^{-6}	2.45076×10^{-7}	309.875	309.8
	3000	0.209997	0.2100	0.177647	9.11062×10^{-7}	1.90878×10^{-7}	338.821	338.7
	3500	0.212369	0.2123	0.180019	6.40017×10^{-7}	1.5657×10^{-7}	365.596	365.5
	4000	0.213579	0.2135	0.18123	4.6925×10^{-7}	1.32807×10^{-7}	390.639	390.5
1	800	0.181131	0.1810	0.148622	0.000185477	0.0000256704	177.497	177.5
	1000	0.184907	0.1848	0.152462	0.000109636	0.0000141262	198.075	198.0
	1500	0.19238	0.1923	0.159993	0.0000434031	5.72341×10^{-6}	241.652	241.5
	2000	0.199466	0.1994	0.167098	0.000022733	3.43735×10^{-6}	278.045	277.9

Table 2 continued

P (atm)	$T\,(K)$	C_P (kJ/kg K)	C_P (kJ/kg K) [19]	C_V (kJ/kg K)	ΔC_P (kJ/kg K)	ΔC_V (kJ/kg K)	u (m/s)	u (m/s) [19]
	2500	0.205819	0.2058	0.173458	0.0000137668	2.45076×10^{-6}	309.935	309.8
	3000	0.210005	0.2100	0.177649	9.11062×10^{-6}	1.90878×10^{-6}	338.88	338.7
	3500	0.212375	0.2123	0.180021	6.40017×10^{-6}	1.5657×10^{-6}	365.654	365.5
	4000	0.213584	0.2135	0.181231	4.6925×10^{-6}	1.32807×10^{-6}	390.695	390.5
10	800	0.182801	0.1810	0.148853	0.00185477	0.000256704	176.773	177.5
	1000	0.185894	0.1848	0.152589	0.00109636	0.000141262	197.95	198.0
	1500	0.192771	0.1923	0.160045	0.000434031	0.0000572341	242.069	241.5
	2000	0.199671	0.1994	0.167129	0.00022733	0.0000343735	278.605	277.9
	2500	0.205943	0.2058	0.17348	0.000137668	0.0000245076	310.531	309.8
	3000	0.210087	0.2100	0.177666	0.0000911062	0.0000190878	339.477	338.7
	3500	0.212433	0.2123	0.180035	0.0000640017	0.000015657	366.239	365.5
	4000	0.213626	0.2135	0.181243	0.000046925	0.0000132807	391.262	390.5

Table 3 The specific heat capacities and speed of sound for UF_2

P (atm)	$T\,(K)$	C_P (kJ/kg K)	C_P (kJ/kg K) [19]	C_V (kJ/kg K)	$\Delta C_P\,(kJ/kg\ K)$	ΔC_V (kJ/kg K)	u (m/ s)	u (m/ s) [19]
0.01	800	0.234206	0.2342	0.204082	1.90783×10^{-6}	2.56011×10^{-7}	166.35	166.3
	1000	0.238873	0.2389	0.208749	1.13324×10^{-6}	1.44351×10^{-7}	185.719	185.7
	1500	0.241806	0.2418	0.211683	4.50789×10^{-7}	6.11084×10^{-8}	227.26	227.2
	2000	0.24136	0.2414	0.211238	2.36265×10^{-7}	3.76152×10^{-8}	262.451	262.4
	2500	0.240328	0.2403	0.210206	1.42933×10^{-7}	2.71861×10^{-8}	293.519	293.4
	3000	0.239016	0.2391	0.208894	9.4406×10^{-8}	2.13394×10^{-8}	321.661	321.6
	3500	0.237864	0.2379	0.207741	6.6149×10^{-8}	1.75858×10^{-8}	347.555	347.4
	4000	0.236866	0.2369	0.206743	4.83508×10^{-8}	1.49602×10^{-8}	371.665	371.5
0.1	800	0.234223	0.2342	0.204084	0.0000190783	2.56011×10^{-6}	166.343	166.3
	1000	0.238883	0.2389	0.208751	0.0000113324	1.44351×10^{-6}	185.718	185.7
	1500	0.24181	0.2418	0.211684	4.50789×10^{-6}	6.11084×10^{-7}	227.265	227.2
	2000	0.241363	0.2414	0.211238	2.36265×10^{-6}	3.76152×10^{-7}	262.458	262.4
	2500	0.24033	0.2403	0.210206	1.42933×10^{-6}	2.71861×10^{-7}	293.526	293.4
	3000	0.239017	0.2391	0.208894	9.4406×10^{-7}	2.13394×10^{-7}	321.668	321.6
	3500	0.237864	0.2379	0.207741	6.6149×10^{-7}	1.75858×10^{-7}	347.562	347.4
	4000	0.236866	0.2369	0.206743	4.83508×10^{-7}	1.49602×10^{-7}	371.672	371.5
1	800	0.234395	0.2342	0.204108	0.000190783	0.0000256011	166.266	166.3
	1000	0.238985	0.2389	0.208764	0.000113324	0.0000144351	185.708	185.7
	1500	0.241851	0.2418	0.211689	0.0000450789	6.11084×10^{-6}	227.316	227.2
	2000	0.241384	0.2414	0.211241	0.0000236265	3.76152×10^{-6}	262.525	262.4

Table 3 continued

P (atm)	$T(K)$	C_P (kJ/kg K)	C_P (kJ/kg K) [19]	C_V (kJ/kg K)	$\Delta C_P (kJ/kg\ K)$	ΔC_V (kJ/kg K)	u(m/s)	u(m/s) [19]
	2500	0.240343	0.2403	0.210209	0.0000142933	2.71861×10^{-6}	293.598	293.4
	3000	0.239026	0.2391	0.208896	9.4406×10^{-6}	2.13394×10^{-6}	321.739	321.6
	3500	0.23787	0.2379	0.207743	6.6149×10^{-6}	1.75858×10^{-6}	347.631	347.4
	4000	0.236871	0.2369	0.206745	4.83508×10^{-6}	1.49602×10^{-6}	371.739	371.5
10	800	0.236112	0.2342	0.204338	0.00190783	0.000256011	165.497	166.3
	1000	0.240005	0.2389	0.208893	0.00113324	0.000144351	185.611	185.7
	1500	0.242256	0.2418	0.211744	0.000450789	0.0000611084	227.828	227.2
	2000	0.241596	0.2414	0.211275	0.000236265	0.0000376152	263.197	262.4
	2500	0.240471	0.2403	0.210233	0.000142933	0.0000271861	294.309	293.4
	3000	0.239111	0.2391	0.208915	0.000094406	0.0000213394	322.449	321.6
	3500	0.23793	0.2379	0.207759	0.000066149	0.0000175858	348.324	347.4
	4000	0.236914	0.2369	0.206758	0.0000483508	0.0000149602	372.409	371.5

Table 4 The specific heat capacities and speed of sound for UF_3

P (atm)	$T\,(K)$	C_P (kJ/kg K)	C_P (kJ/kg K) [19]	C_V (kJ/kg K)	ΔC_P (kJ/kg K)	ΔC_V (kJ/kg K)	u (m/s)	u (m/s) [19]
0.01	800	0.27825	0.2783	0.250066	1.93292×10^{-6}	2.5262×10^{-7}	158.439	158.4
	1000	0.281851	0.2820	0.253667	1.15346×10^{-6}	1.4633×10^{-7}	177.013	177.0
	1500	0.293804	0.2937	0.265621	4.60765×10^{-7}	6.48762×10^{-8}	216.308	216.2
	2000	0.30694	0.3070	0.278758	2.41508×10^{-7}	4.09209×10^{-8}	249.206	249.1
	2500	0.31753	0.3176	0.289347	1.45859×10^{-7}	2.99609×10^{-8}	278.153	278.1
	3000	0.323905	0.3240	0.295723	9.60816×10^{-8}	2.36879×10^{-8}	304.409	304.3
	3500	0.326725	0.3266	0.298542	6.70966×10^{-8}	1.96041×10^{-8}	328.664	328.6
	4000	0.326409	0.3265	0.298226	4.88503×10^{-8}	1.67203×10^{-8}	351.373	351.3
0.1	800	0.278267	0.2783	0.250068	0.0000193292	2.5262×10^{-6}	158.432	158.4
	1000	0.281861	0.2820	0.253668	0.0000115346	1.4633×10^{-6}	177.014	177.0
	1500	0.293808	0.2937	0.265622	4.60765×10^{-6}	6.48762×10^{-7}	216.315	216.2
	2000	0.306942	0.3070	0.278758	2.41508×10^{-6}	4.09209×10^{-7}	249.214	249.1
	2500	0.317531	0.3176	0.289347	1.45859×10^{-6}	2.99609×10^{-7}	278.161	278.1
	3000	0.323906	0.3240	0.295723	9.60816×10^{-7}	2.36879×10^{-7}	304.417	304.3
	3500	0.326725	0.3266	0.298543	6.70966×10^{-7}	1.96041×10^{-7}	328.672	328.6
	4000	0.326409	0.3265	0.298227	4.88503×10^{-7}	1.67203×10^{-7}	351.38	351.3
1	800	0.278441	0.2783	0.250091	0.000193292	0.000025262	158.364	158.4
	1000	0.281965	0.2820	0.253682	0.000115346	0.000014633	177.016	177.0
	1500	0.29385	0.2937	0.265628	0.0000460765	6.48762×10^{-6}	216.381	216.2
	2000	0.306964	0.3070	0.278762	0.0000241508	4.09209×10^{-6}	249.295	249.1

Table 4 continued

P (atm)	$T\,(K)$	C_P (kJ/kg K)	C_P (kJ/kg K) [19]	C_V (kJ/kg K)	ΔC_P (kJ/kg K)	ΔC_V (kJ/kg K)	u (m/s)	u (m/s) [19]
	2500	0.317544	0.3176	0.28935	0.0000145859	2.99609×10^{-6}	278.245	278.1
	3000	0.323915	0.3240	0.295725	9.60816×10^{-6}	2.36879×10^{-6}	304.5	304.3
	3500	0.326731	0.3266	0.298544	6.70966×10^{-6}	1.96041×10^{-6}	328.753	328.6
	4000	0.326414	0.3265	0.298228	4.88503×10^{-6}	1.67203×10^{-6}	351.458	351.3
10	800	0.280181	0.2783	0.250318	0.00193292	0.00025262	157.681	158.4
	1000	0.283003	0.2820	0.253813	0.00115346	0.00014633	177.046	177.0
	1500	0.294264	0.2937	0.265686	0.000460765	0.0000648762	217.036	216.2
	2000	0.307182	0.3070	0.278799	0.000241508	0.0000409209	250.103	249.1
	2500	0.317675	0.3176	0.289377	0.000145859	0.0000299609	279.082	278.1
	3000	0.324001	0.3240	0.295747	0.0000960816	0.0000236879	305.328	304.3
	3500	0.326792	0.3266	0.298562	0.0000670966	0.0000196041	329.556	328.6
	4000	0.326458	0.3265	0.298243	0.0000488503	0.0000167203	352.232	351.3

Table 5 The specific heat capacities and speed of sound for UF_4

P (atm)	$T\,(K)$	C_P (kJ/kg K)	C_P (kJ/kg K) [19]	C_V (kJ/kg K)	ΔC_P (kJ/kg K)	ΔC_V (kJ/kg K)	u (m/s)	u (m/s) [19]
0.01	800	0.349765	0.3498	0.323286	1.9274×10^{-6}	2.47027×10^{-7}	151.43	151.4
	1000	0.354571	0.3548	0.328093	1.15509×10^{-6}	1.47378×10^{-7}	169.211	169.2
	1500	0.364196	0.3644	0.337718	4.62991×10^{-7}	6.8538×10^{-8}	207.02	206.9
	2000	0.371681	0.3717	0.345203	2.42494×10^{-7}	4.42643×10^{-8}	238.858	238.8
	2500	0.376241	0.3764	0.349763	1.46083×10^{-7}	3.28016×10^{-8}	266.927	266.8
	3000	0.378566	0.3788	0.352089	9.58813×10^{-8}	2.6104×10^{-8}	292.336	292.2
	3500	0.379505	0.3793	0.353028	6.66613×10^{-8}	2.16846×10^{-8}	315.729	315.6
	4000	0.378566	0.3786	0.352089	4.82852×10^{-8}	1.85361×10^{-8}	337.56	337.5
0.1	800	0.349782	0.3498	0.323288	0.000019274	2.47027×10^{-6}	151.425	151.4
	1000	0.354582	0.3548	0.328094	0.0000115509	1.47378×10^{-6}	169.213	169.2
	1500	0.3642	0.3644	0.337719	4.62991×10^{-6}	6.8538×10^{-7}	207.029	206.9
	2000	0.371683	0.3717	0.345204	2.42494×10^{-6}	4.42643×10^{-7}	238.868	238.8
	2500	0.376242	0.3764	0.349764	1.46083×10^{-6}	3.28016×10^{-7}	266.937	266.8
	3000	0.378567	0.3788	0.352089	9.58813×10^{-7}	2.6104×10^{-7}	292.346	292.2
	3500	0.379506	0.3793	0.353028	6.66613×10^{-7}	2.16846×10^{-7}	315.739	315.6
	4000	0.378567	0.3786	0.352089	4.82852×10^{-7}	1.85361×10^{-7}	337.569	337.5
1	800	0.349955	0.3498	0.32331	0.00019274	0.0000247027	151.373	151.4
	1000	0.354685	0.3548	0.328108	0.000115509	0.0000147378	169.234	169.2
	1500	0.364241	0.3644	0.337725	0.0000462991	6.8538×10^{-6}	207.113	206.9
	2000	0.371705	0.3717	0.345208	0.0000242494	4.42643×10^{-6}	238.966	238.8

Table 5 continued

P (atm)	$T\,(K)$	C_P (kJ/kg K)	C_P (kJ/kg K) [19]	C_V (kJ/kg K)	ΔC_P (kJ/kg K)	ΔC_V (kJ/kg K)	u (m/s)	u (m/s) [19]
	2500	0.376255	0.3764	0.349767	0.0000146083	3.28016×10^{-6}	267.037	266.8
	3000	0.378576	0.3788	0.352092	9.58813×10^{-6}	2.6104×10^{-6}	292.443	292.2
	3500	0.379512	0.3793	0.35303	6.66613×10^{-6}	2.16846×10^{-6}	315.833	315.6
	4000	0.378571	0.3786	0.352091	4.82852×10^{-6}	1.85361×10^{-6}	337.66	337.5
10	800	0.35169	0.3498	0.323533	0.0019274	0.000247027	150.851	151.4
	1000	0.355725	0.3548	0.32824	0.00115509	0.000147378	169.442	169.2
	1500	0.364658	0.3644	0.337787	0.000462991	0.000068538	207.95	206.9
	2000	0.371923	0.3717	0.345248	0.000242494	0.0000442643	239.946	238.8
	2500	0.376387	0.3764	0.349796	0.000146083	0.0000328016	268.035	266.8
	3000	0.378662	0.3788	0.352115	0.0000958813	0.0000958813	293.419	292.2
	3500	0.379572	0.3793	0.35305	0.0000666613	0.0000216846	316.774	315.6
	4000	0.378614	0.3786	0.352108	0.0000482852	0.0000185361	338.563	337.5

Table 6 The specific heat capacities and speed of sound for UF_5

P (atm)	$T\,(K)$	C_P (kJ/kg K)	C_P (kJ/kg K) [19]	C_V (kJ/kg K)	ΔC_P (kJ/kg K)	ΔC_V (kJ/kg K)	u (m/s)	u (m/s) [19]
0.01	800	0.39594	0.3958	0.370972	1.89024×10^{-6}	2.39906×10^{-7}	146.051	146.0
	1000	0.402674	0.4029	0.377706	1.13719×10^{-6}	1.47827×10^{-7}	163.199	163.1
	1500	0.410846	0.4111	0.385879	4.56909×10^{-7}	7.21962×10^{-8}	199.747	199.7
	2000	0.415677	0.4154	0.39071	2.3887×10^{-7}	4.7693×10^{-8}	230.561	230.5
	2500	0.418138	0.4182	0.393172	1.43361×10^{-7}	3.57355×10^{-8}	257.726	257.6
	3000	0.420004	0.4198	0.395038	9.36283×10^{-8}	2.86046×10^{-8}	282.285	282.2
	3500	0.420004	0.4203	0.395038	6.47087×10^{-8}	2.38389×10^{-8}	304.903	304.8
	4000	0.420004	0.4200	0.395038	4.65497×10^{-8}	2.04158×10^{-8}	325.954	325.9
0.1	800	0.395957	0.3958	0.370974	0.0000189024	2.39906×10^{-6}	146.049	146.0
	1000	0.402684	0.4029	0.377708	0.0000113719	1.47827×10^{-6}	163.204	163.1
	1500	0.41085	0.4111	0.38588	4.56909×10^{-6}	7.21962×10^{-7}	199.758	199.7
	2000	0.415679	0.4154	0.390711	2.3887×10^{-6}	4.7693×10^{-7}	230.573	230.5
	2500	0.418139	0.4182	0.393172	1.43361×10^{-6}	3.57355×10^{-7}	257.738	257.6
	3000	0.420005	0.4198	0.395038	9.36283×10^{-7}	2.86046×10^{-7}	282.297	282.2
	3500	0.420005	0.4203	0.395038	6.47087×10^{-7}	2.38389×10^{-7}	304.914	304.8
	4000	0.420005	0.4200	0.395038	4.65497×10^{-7}	2.04158×10^{-7}	325.965	325.9
1	800	0.396127	0.3958	0.370996	0.000189024	0.0000239906	146.026	146.0
	1000	0.402786	0.4029	0.377721	0.000113719	0.0000147827	163.253	163.1
	1500	0.410891	0.4111	0.385886	0.0000456909	7.21962×10^{-6}	199.866	199.7
	2000	0.415701	0.4154	0.390715	0.000023887	4.7693×10^{-6}	230.692	230.5

Table 6 continued

P (atm)	$T(K)$	C_P (kJ/kg K)	C_P (kJ/kg K) [19]	C_V (kJ/kg K)	ΔC_P (kJ/kg K)	ΔC_V (kJ/kg K)	u (m/s)	u (m/s) [19]
	2500	0.418152	0.4182	0.393175	0.0000143361	3.57355×10^{-6}	257.857	257.6
	3000	0.420014	0.4198	0.395041	9.36283×10^{-6}	2.86046×10^{-6}	282.412	282.2
	3500	0.420011	0.4203	0.39504	6.47087×10^{-6}	2.38389×10^{-6}	305.024	304.8
	4000	0.420009	0.4200	0.39504	4.65497×10^{-6}	2.04158×10^{-6}	326.07	325.9
10	800	0.397828	0.3958	0.371212	0.00189024	0.000239906	145.801	146.0
	1000	0.40381	0.4029	0.377854	0.00113719	0.000147827	163.739	163.1
	1500	0.411303	0.4111	0.385951	0.000456909	0.0000721962	200.943	199.7
	2000	0.415916	0.4154	0.390758	0.00023887	0.000047693	231.883	230.5
	2500	0.418281	0.4182	0.393207	0.000143361	0.0000357355	259.043	257.6
	3000	0.420098	0.4198	0.395066	0.0000936283	0.0000286046	283.558	282.2
	3500	0.420069	0.4203	0.395062	0.0000647087	0.0000238389	306.121	304.8
	4000	0.420051	0.4200	0.395058	0.0000465497	0.0000204158	327.118	325.9

Table 7 The specific heat capacities and speed of sound for UF_6

P (atm)	$T\,(K)$	C_P (kJ/kg K)	C_P (kJ/kg K) [19]	C_V (kJ/kg K)	ΔC_P (kJ/kg K)	ΔC_V (kJ/kg K)	u (m/ s)	u (m/ s) [19]
0.01	800	0.433669	0.4338	0.410048	1.81974×10^{-6}	2.31921×10^{-7}	141.408	141.4
	1000	0.438713	0.4390	0.415093	1.09838×10^{-6}	1.47934×10^{-7}	158.048	158.0
	1500	0.444631	0.4444	0.421012	4.41744×10^{-7}	7.58621×10^{-8}	193.495	193.4
	2000	0.446137	0.4463	0.422518	2.30169×10^{-7}	5.11769×10^{-8}	223.408	223.3
	2500	0.446894	0.4472	0.423276	1.37389×10^{-7}	3.87241×10^{-8}	249.765	249.7
	3000	0.446894	0.4477	0.423276	8.91119×10^{-8}	3.11518×10^{-8}	273.604	273.5
	3500	0.447654	0.4479	0.424035	6.10858×10^{-8}	2.60313×10^{-8}	295.512	295.4
	4000	0.448417	0.4481	0.424798	4.35291×10^{-8}	2.23263×10^{-8}	315.9	315.8
0.1	800	0.433685	0.4338	0.41005	0.0000181974	2.31921×10^{-6}	141.41	141.4
	1000	0.438722	0.4390	0.415094	0.0000109838	1.47934×10^{-6}	158.056	158.0
	1500	0.444635	0.4444	0.421013	4.41744×10^{-6}	7.58621×10^{-7}	193.509	193.4
	2000	0.446139	0.4463	0.422519	2.30169×10^{-6}	5.11769×10^{-7}	223.422	223.3
	2500	0.446896	0.4472	0.423276	1.37389×10^{-6}	3.87241×10^{-7}	249.779	249.7
	3000	0.447655	0.4477	0.424036	8.91119×10^{-7}	3.11518×10^{-7}	273.605	273.5
	3500	0.447655	0.4479	0.424036	6.10858×10^{-7}	2.60313×10^{-7}	295.525	295.4
	4000	0.448417	0.4481	0.424798	4.35291×10^{-7}	2.23263×10^{-7}	315.913	315.8
1	800	0.433849	0.4338	0.410071	0.000181974	0.0000231921	141.428	141.4
	1000	0.438821	0.4390	0.415107	0.000109838	0.0000147934	158.141	158.0
	1500	0.444675	0.4444	0.42102	0.0000441744	7.58621×10^{-6}	193.646	193.4
	2000	0.44616	0.4463	0.422523	0.0000230169	5.11769×10^{-6}	223.566	223.3

Table 7 continued

P (atm)	$T\,(K)$	C_P (kJ/kg K)	C_P (kJ/kg K) [19]	C_V (kJ/kg K)	ΔC_P (kJ/kg K)	ΔC_V (kJ/kg K)	u (m/s)	u (m/s) [19]
	2500	0.446908	0.4472	0.423279	0.0000137389	3.87241×10^{-6}	249.92	249.7
	3000	0.447663	0.4477	0.424039	8.91119×10^{-6}	3.11518×10^{-6}	273.739	273.5
	3500	0.44766	0.4479	0.424038	6.10858×10^{-6}	2.60313×10^{-6}	295.652	295.4
	4000	0.448421	0.4481	0.4248	4.35291×10^{-6}	2.23263×10^{-6}	316.033	315.8
10	800	0.435487	0.4338	0.41028	0.00181974	0.000231921	141.61	141.4
	1000	0.43981	0.4390	0.415241	0.00109838	0.000147934	158.988	158.0
	1500	0.445072	0.4444	0.421088	0.000441744	0.0000758621	195.011	193.4
	2000	0.446367	0.4463	0.422569	0.000230169	0.0000511769	225.0	223.3
	2500	0.447032	0.4472	0.423314	0.000137389	0.0000387241	251.319	249.7
	3000	0.447743	0.4477	0.424067	0.0000891119	0.0000311518	275.076	273.5
	3500	0.447715	0.4479	0.424061	0.0000610858	0.0000260313	296.923	295.4
	4000	0.44846	0.4481	0.42482	0.0000435291	0.0000223263	317.24	315.8

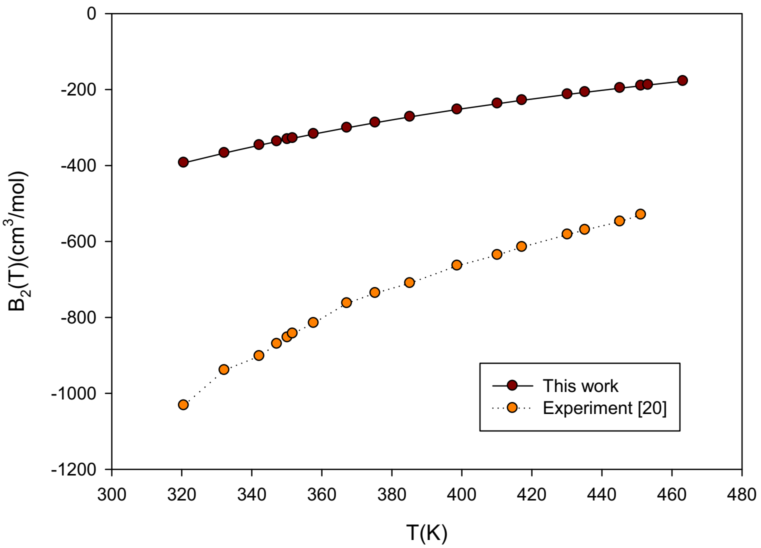

Fig. 1 The temperature dependence of the second virial coefficient of UF_6 and its comparison with experimental data

Table 8 Lennard-Jones (12-6) potential parameters and molecular mass

Molecules	$\sigma(A^\circ)$	$\varepsilon/k_B(K)$	Molecular mass (Kg/Kmol)
U	4.531	1266	238
UF	4.400	377.5	257
UF_2	4.713	349.4	276
UF_3	5.027	321.2	295
UF_4	5.340	293.1	314
UF_5	5.654	264.9	333
UF_6	5.967	236.8	352

For heat capacity at constant volume

$$C_V - C_V^0 = -\frac{P}{T}\left(2B^{'}\left(T^*\right) + B^{''}\left(T^*\right)\right), \tag{5}$$

For heat capacity at constant pressure

$$C_P - C_P^0 = -\frac{PB^{''}(T^*)}{T} + \frac{P^2\left(B(T^*) - B^{'}(T^*)\right)^2}{RT^2}, \tag{6}$$

For speed of sound

$$u^2 = \frac{\gamma RT}{M}\left[1 + \frac{P}{RT}\left(2B\left(T^*\right) + 2(\gamma - 1)B^{'}\left(T^*\right) + \frac{(\gamma - 1)^2}{\gamma}B^{''}\left(T^*\right)\right)\right]. \tag{7}$$

here, $B^{'}(T^*) = T^*\left(\mathrm{d}B(T^*)/\mathrm{d}T^*\right)$ and $B^{''}(T^*) = T^{*2}\left(\mathrm{d}^2B(T^*)/\mathrm{d}T^{*2}\right)$ are first and second derivatives of Eq. (4), respectively.

3 Numerical results and discussion

In this work, new analytical formulae have been presented to evaluate the specific heat capacities and speed of sound of nuclear material gases. Furthermore, the presented analytical formulae can be useful to calculate other thermodynamic properties of all gases. The Mathematica 7.0 international mathematical software was used to calculate the analytical formulae obtained for the specific heat capacities and speed of sound in this paper. It is well known that the thermodynamic properties of real gases are defined with virial coefficients. Note that, at low densities, the deviations from the ideal state are adequately explained by the second virial coefficient, but at higher densities, higher virial coefficients such as third, fourth and fifty virial coefficients must be taken into account [15]. The accuracy of virial coefficients is critical to proper description of the metastable region because of the multiplicative effect of virial coefficients error on the thermodynamic property accuracy (e.g., specific heat capacity and speed of sound from virial equation of state), increasing progressively with density [16]. Therefore, the heat capacities and speed of sound of gases can be written in terms of the second virial coefficient at low densities. It is well known that the real gases begin to passing the liquid phase at low temperatures and high pressures. Therefore, as seen in Tables 1, 2, 3, 4, 5, 6 and 7 at low temperatures and high pressures, the calculation results obtained from the heat capacities using the second virial coefficient deviate from the literature data [17]. The speed of sound and specific heat capacities of important nuclear gases of U, UF, UF_2, UF_3, UF_4, UF_5 and UF_6 were determined in the temperature range from 800 K to 4000 K and pressure range from 0.01 atm to 10 atm. The quantities ΔC_P and ΔC_V correspond to $C_P - C_P^0$ and $C_V - C_V^0$, respectively. To show the accuracy and precision of the analytical formulae, we present several calculations of the specific heat capacity and speed of sound of gases of U, UF, UF_2, UF_3, UF_4, UF_5 and UF_6 various pressure and temperature range. The calculation results of the specific heat capacity and speed of sound of gases of U, UF, UF_2, UF_3, UF_4, UF_5 and UF_6 are given in Tables 1, 2, 3, 4, 5, 6 and 7. As can be seen from Tables 1, 2, 3, 4, 5, 6 and 7, the obtained results of specific heat capacities and speed of sound for uranium and uranium fluoride gases are in a good agreement with theoretical data, especially at low pressure (0.01 atm to 10 atm) [18, 19]. The results of the analytical formula for second virial coefficient and experimental data [20] of UF_6 are plotted in Fig. 1. As seen from Fig. 1, our results are approximately agreed with the experimental data. The consistency of results demonstrates that the proposed analytical expressions are applicable for uranium and uranium fluoride gases. The Lennard-Jones parameters and molecular mass of nuclear gases are given in Table 8 [21].

4 Conclusions

In this study, taking the second virial coefficient with Lennard-Jones potential (12-6) into consideration has been derived into explicit and efficiently analytical formulae for the specific heat capacities and speed of sound. The results from the analytical formulae for uranium and uranium fluoride gases are in good agreement with the literature data. These gases are widely used in the nuclear industry for gaseous diffusion, the process of enriching uranium, energy production. In conclusion, in certain temperature and pressure ranges, the analytical formulae offer the advantage of direct and precise calculation of the specific heat capacities and speed of sound.

Acknowledgements This work has been supported by the Scientific and Technological Research Council of Turkey (TUBITAK) Science Fellowships and Grant Programmes Department (BIDEB).

References

1. D.A. McQuarine, *Statistical Mechanics* (Harper & Row, New York, 1973), pp. 224–236
2. L.D. Landau, E.M. Lifshitz, *Statistical Physics* (Addison-W, London, 1969), pp. 237–241
3. Thermophysical Properties of Materials for Nuclear Engineering: A Tutorial and Collection of Data. Int. Atomic Energy Agency, Vienna (2008)
4. R. Dewitt, *Uranium Hexafluaride: A Survey of the Physico-Chemical Properties* (Goodyear Atomic Corporation, Ohio, 1960)
5. M.S. Van Den Berg, Ann. Nucl. Energy **22**(9), 562–584 (1995)
6. K. Masao, S. Werner, S. Darwin, W. Bernard, J. Chem. Phys. **48**(8), 4001–4012 (1968)
7. J. Emsley, *Uranium Nature's Building Blocks: An A to Z Guide to the Elements* (Oxford University Press, Oxford, 2001), pp. 476–482
8. G.T., Seaborg, Uranium. The Encyclopedia of the Chemical Elements. Skokie, Illinois: Reinhold Book Corporation. pp. 773–786. LCCCN 68-29938 (1968)
9. C.B. Jeff, Introduction to Nuclear Science, 1st ed. Boca Raton, (January 8, 2016) (FL, U.S.A: CRC Press, 2009)
10. C.B. Jeff, Introduction to Nuclear Science, 1st ed. Boca Raton, (June 17, 2015) (FL, U.S.A: CRC Press, 2009)
11. A. Harmens, H. Knapp. Ind. Eng. Chem. Fund. 19291–294 (1980)
12. S. Lee, J. Jeon, W. Kim, T.S. Chair, J. Phys. Chem. B **112**, 15725–15741 (2008)
13. J.O. Hirschfelder, C.F. Curtiss, R.B. Bird, *Molecular Theory of Gases and Liquids* (Wiley, New York, 1954), pp. 326–354
14. E. Somuncu, J. Indian Phys. (2018). https://doi.org/10.1007/s12648-018-1334-x
15. A. Hutem, S. Boonchui, J. Math. Chem. **50**, 1262–1276 (2012)
16. M. Duska, J. Hruby, J, EPJ Web of Conferences 45, 01024 (2013)
17. C. Guder, W. Wagner, J. Phys. Chem. Ref. Data **38**, 33–94 (2009)
18. H.A. Hassan, J.E. Deese, Thermodynamic properties of UF_6 at High Temperatures, Nasa Contractor Report, Nasa Cr-2373 (1974)
19. CEARUN, NASA, https://cearun.grc.nasa.gov [retrieved 2015]
20. J.H. Dymond, K.N. Marsh, R.C. Wilhoit, K.C. Wong, *Virial Coefficients of Pure Gases and Mixtures* (Springer Verlag, Berlin, 2002)
21. M.S. Van Den Berg, Ann. Nucl. Energy **22**, 565–584 (1954)