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Assessment of Three Databases for the NASA Seven-Coefficient Polynomial Fits for Calculating Thermodynamic Properties of Individual Species

Research Article

Appendix: Polynomial Coefficients

Table 11. Polynomial coefficients for molecular oxygen (O_2).

Database	GRI		OpenFOAM		Burcat	
T_{low} (K)	200		200		200	
T_{High} (K)	3,500		5,000		6,000	
T_{common} (K)	1,000		1,000		1,000	
T interval	high-T	low-T	high-T	low-T	high-T	low-T
a_1	3.28253784	3.78245636	3.6975780	3.2129360	3.66096065	3.78245636
10^3 a_2	1.48308754	-2.99673416	0.61351970	1.1274860	0.656365811	-2.99673416
10^6 a_3	-0.757966669	9.84730201	-0.12588420	-0.5756150	-0.141149627	9.84730201
10^9 a_4	0.209470555	-9.68129509	0.017752810	1.3138770	0.020579794	-9.68129509
10^{12} a_5	-0.021671779	3.24372837	-0.0011364350	-0.87685540	-0.00129913436	3.24372837
10^{-3} a_6	-1.08845772	-1.06394356	-1.233930	-1.0052490	-1.21597718	-1.06394356
a_7	5.45323129	3.65767573	3.1891660	6.0347380	3.41536279	3.65767573

Table 12. Polynomial coefficients for molecular nitrogen (N_2).

Database	GRI		OpenFOAM		Burcat	
T_{low} (K)	300		200		200	
T_{High} (K)	5,000		5,000		6,000	
T_{common} (K)	1,000		1,000		1,000	
T interval	high-T	low-T	high-T	low-T	high-T	low-T
a_1	2.926640	3.2986770	2.926640	3.2986770	2.95257637	3.53100528
10^3 a_2	1.48797680	1.40824040	1.4879770	1.408240	1.39690040	-0.123660988
10^6 a_3	-0.5684760	-3.9632220	-0.56847610	-3.9632220	-0.492631603	-0.502999433
10^9 a_4	0.100970380	5.6415150	0.10097040	5.6415150	0.07860102	2.43530612
10^{12} a_5	-0.0067533510	-2.4448540	-0.006753351	-2.4448550	-0.004607552	-1.40881235
10^{-3} a_6	-0.92279770	-1.02089990	-0.92279770	-1.02090	-0.923948688	-1.04697628
a_7	5.9805280	3.9503720	5.9805280	3.9503720	5.87188762	2.96747038

***Corresponding Author**:
Osama A. Marzouk,
Assistant Professor, College of Engineering, University of Buraimi, P.O. Box 890, Post Code 512, Al Buraimi, Sultanate of Oman, Oman.
Email: osama.m@uob.edu.om

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Table 13. Polynomial coefficients for molecular hydrogen (H_2).

Database	GRI		OpenFOAM		Burcat	
T_{low} (K)	200		200		200	
T_{High} (K)	3,500		5,000		6,000	
T_{common} (K)	1,000		1,000		1,000	
T interval	high-T	low-T	high-T	low-T	high-T	low-T
a_1	3.33727920	2.34433112	2.9914230	3.2981240	2.93286575	2.34433112
10^3 a_2	-0.0494024731	7.98052075	0.70006440	0.82494420	0.826608026	7.98052075
10^6 a_3	0.499456778	-19.4781510	-0.056338290	-0.81430150	-0.146402364	-19.4781510
10^9 a_4	-0.179566394	20.1572094	-0.009231578	-0.094754340	0.0154100414	20.1572094
10^{12} a_5	0.0200255376	-7.37611761	0.0015827520	0.41348720	-0.0006888048	-7.37611761
10^{-3} a_6	-0.950158922	-0.917935173	-0.8350340	-1.0125210	-0.813065581	-0.917935173
a_7	-3.20502331	0.683010238	-1.355110	-3.2940940	-1.024328650	0.683010238

Table 14. Polynomial coefficients for methane (CH_4).

Database	GRI		OpenFOAM		Burcat	
T_{low} (K)	200		200		200	
T_{High} (K)	3,500		5,000		6,000	
T_{common} (K)	1,000		1,462		1,000	
T interval	high-T	low-T	high-T	low-T	high-T	low-T
a_1	0.074851495	5.14987613	4.096176530	3.72113020	1.9117860	5.148257320
10^3 a_2	13.39094670	-13.67097880	7.443308450	-2.502932890	9.60267960	-13.7002410
10^6 a_3	-5.732858090	49.1800599	-2.6387190	19.02465340	-3.383878410	49.37494140
10^9 a_4	1.222925350	-48.4743026	0.495776040	-14.6871253	0.538797240	-49.1952339
10^{12} a_5	-0.101815230	16.6693956	-0.024750805	3.437911520	-0.03193068107	17.0097299
10^{-3} a_6	-9.46834459	-10.2466476	-11.3835704	-10.1424099	-10.0992136	-10.2453222
a_7	18.4373180	-4.641303760	-4.675613830	1.227765960	8.482418610	-4.633227260

Table 15. Polynomial coefficients for carbon dioxide (CO_2).

Database	GRI		OpenFOAM		Burcat	
T_{low} (K)	200		200		200	
T_{High} (K)	3,500		5,000		6,000	
T_{common} (K)	1,000		1,380		1,000	
T interval	high-T	low-T	high-T	low-T	high-T	low-T
a_1	3.857460290	2.356773520	5.189530180	2.57930490	4.63651110	2.3568130
10^3 a_2	4.414370260	8.984596770	2.060064760	8.246849870	2.74145690	8.98412990
10^6 a_3	-2.214814040	-7.123562690	-0.733575324	-6.427160470	-0.995897590	-7.12206320
10^9 a_4	0.523490188	2.459190220	0.117004374	2.546370240	0.160386660	2.45730080
10^{12} a_5	-0.047208416	-0.143699548	-0.006917292	-0.412030443	-0.009161986	-0.142885480
10^{-3} a_6	-48.75916600	-48.37196970	-49.31789530	-48.4162830	-49.0249040	-48.3719710
a_7	2.27163806	9.901052220	-5.182893030	8.811410410	-1.93489550	9.90090350

Table 16. Polynomial coefficients for water vapor (H_2O).

Database	GRI		OpenFOAM		Burcat	
T_{low} (K)	200		200		200	
T_{High} (K)	3,500		5,000		6,000	
T_{common} (K)	1,000		1,000		1,000	
T interval	high-T	low-T	high-T	low-T	high-T	low-T
a_1	3.033992490	4.198640560	2.6721460	3.3868420	2.67703890	4.19863520
$10^3 a_2$	2.176918040	-2.03643410	3.0562930	3.4749820	2.97318160	-2.03640170
$10^6 a_3$	-0.164072518	6.520402110	-0.8730260	-6.3546960	-0.773768890	6.52034160
$10^9 a_4$	-0.097041987	-5.487970620	0.12009960	6.9685810	0.094433514	-5.48792690
$10^{12} a_5$	0.016820099	1.771978170	-0.006391618	-2.5065880	-0.0042689991	1.7719680
$10^{-3} a_6$	-30.00429710	-30.29372670	-29.899210	-30.208110	-29.8858940	-30.2937260
a_7	4.96677010	-0.849032208	6.8628170	2.5902330	6.882550	-0.84900901