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Rational approximations

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Abstract

A computer algorithm and software is presented here. The software provides a rational or polynomial approximation for a giving data set. The software runs on Macintosh OS X; a copy can be obtained from the authors.

Keywords: Rational approximation; Thermophysical properties; SOFC modeling

1. Introduction

A rational approximation is defined as the ratio of two polynomials:

$$R(x) = \frac{P(x)}{Q(x)} = \frac{\sum_{i=1}^{N} a_i x^i}{1 + \sum_{i=1}^{M} b_i x^i} = p\left[\frac{N}{M}\right].$$

The coefficients a_i and b_i can be determined using the least squares error method:[1]

$$\mathrm{LSE} = \sum_{i=0}^{k}\left(f_i\left(1 + \sum_{j=1}^{M} b_j x^j\right) - \sum_{j=1}^{N} a_j x^j\right)^2,$$
$$\frac{\partial(\mathrm{LSE})}{\partial a_j} = 0, \quad \frac{\partial(\mathrm{LSE})}{\partial b_j} = 0$$

The resulting equations once expressed in matrix form can be readily solved with conventional linear algebra methods. Rational approximations are used for representing complicated structures, for either interpolation or extrapolation, and usually require less fitting parameters than polynomials do.

2. Algorithm

An algorithm for calculating the rational approximation is presented in this section. The algorithm focuses in constructing the coefficient matrix, the actual solution to this matrix is not discussed because it can be found in any linear algebra textbook. Four different sub-matrices are constructed first and then the final matrix is composed from these sub-matrices. The algorithm is presented in *pseudo-code*.

This pseudo-code can be easily transported to any computer language. Do notice, however, that $p[N/M]$ is a class of Padé type. Defining a class of Padé type results in a simpler and more elegant code. Nevertheless, this variable can be substituted by an **Array** type.

3. Features

A small guide describing the functionality of the software is presented in this section. The software, named **Padé**, was created for generating rational approximations to important fluids in solid oxide fuel cells [1].

Padé is a versatile application for curve fitting. It provides an easy way to calculate rational approximations, seldom to find in mathematical software, and at the same time it can generate polynomial approximations. A polynomial approximation ($p[N/0]$) is a special case of a more general family of functions called rational functions ($p[N/M]$).

The **Padé's** main window opens after the software is launched; one click in the presentation window will activate the main window. The basic components of the main window are (see Fig. 1):

1. The degree of the rational function: `Padé[N/M]`
2. The input data field: `Data:`
3. The data-box

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[1] The squared error $E = (f(x) - P(x)/Q(x))^2$ will produce a set of non-linear equations, however, an alternative linear form was proposed by Cauchy–Padé ($E = (f(x)Q(x) - P(x)^2)$).

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$\mathbf{A}\times\mathbf{c_f}=\mathbf{B}$ //This algorithm constructs matrices **A, B**.

// The solution to the equation above determines the fitting paramenters: $\mathbf{c_f}$

dim $p[N/M]$ **Pade type**

input-data x, y;

$p[N/M]$.datax $\leftarrow x$;

$p[N/M]$.datay $\leftarrow y$;

  for row=0 to $N+M$

  for col=0 to $N+M$

    if (col$\leq N$) **and** (row$\leq N$) { A(row,col)=-$\sum_{i=0}^{k}(p[N/M].\text{datax})^{\text{row+col}}$ };

    if (col$> N$) **and** (row$\leq N$) { A(row,col)=$\sum_{i=0}^{k} p[N/M].\text{datay}\times(p[N/M].\text{datax})^{\text{row+col}-N}$ };

    if (col$\leq N$) **and** (row$> N$) { A(row,col)=-$\sum_{i=0}^{k} p[N/M].\text{datay}\times(p[N/M].\text{datax})^{\text{row+col}-N}$ };

    if (col$> N$) **and** (row$> N$) { A(row,col)=$\sum_{i=0}^{k}(p[N/M].\text{datay})^2\times(p[N/M].\text{datax})^{\text{row+col}-2N}$ };

  next col

    If (row$\leq N$) { B(row)=-$\sum_{i=0}^{k} p[N/M].\text{datay}\times(p[N/M].\text{datax})^{\text{row}}$ };

    if (row$> N$) { B(row)=-$\sum_{i=0}^{k}(p[N/M].\text{datay})^2\times(p[N/M].\text{datax})^{\text{row-N}}$ };

  next row

// Solution:

$p[N/M].\mathbf{c_f}=\mathbf{A}^{-1}\times\mathbf{B}$

4. The buttons section: `Confirm data`, `Coefficients`, `Calculate`, `Remove Row`, `Matrices`, `Delete`, `Plot Results`

3.1. Data field

Basically, there are two ways the user can input data: (1) through the data field named `Data:` in the main window; and (2) through the `Open` ... command in the `File` menu bar. If the data set is small, we suggest to use the data field in the main window, otherwise a pre-saved data set will be more convenient. The data is entered in two steps, first the value for the independent variable (x) and secondly the value for the dependent variable (y). After the data set is completed, the user has the option to store the information for later use, this is accomplished using the `Save` ... command in the

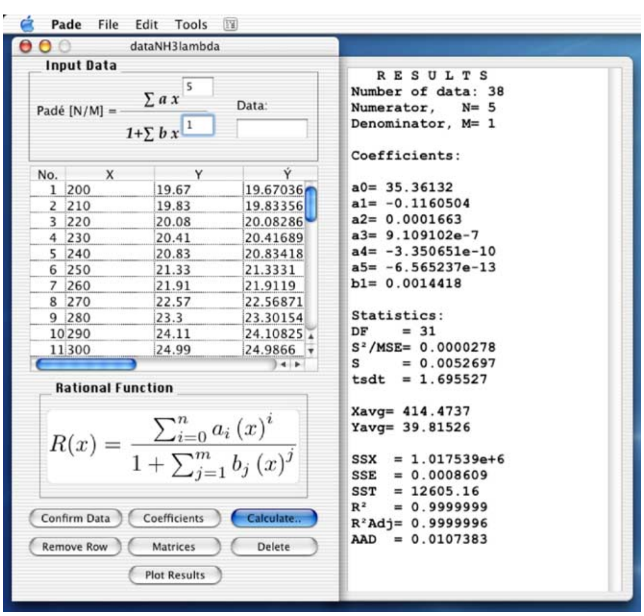

Fig. 1. Main window.

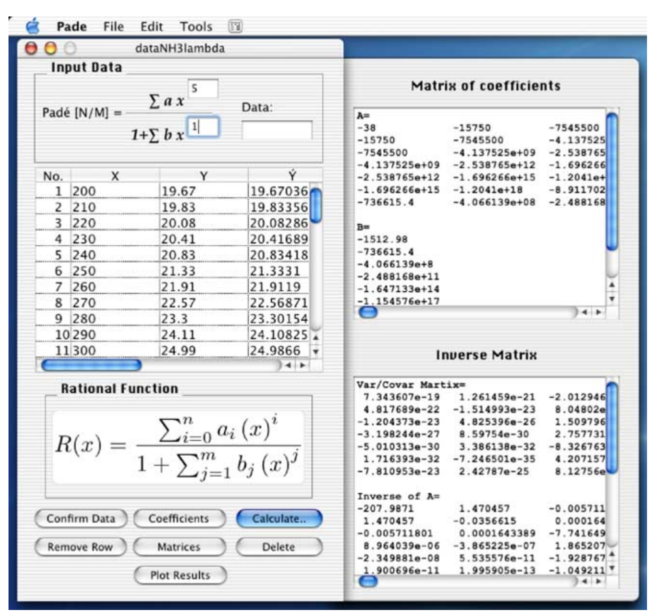

Fig. 2. Matrices window.

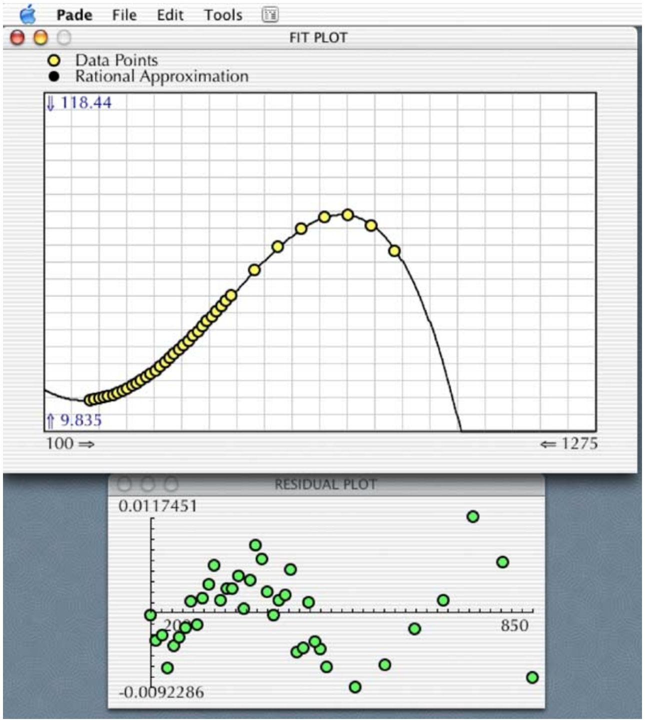

Fig. 3. Rational approximation and residual plot windows.

`File` menu bar. When using pre-saved data sets the data has to be saved as a *tab-delimited* file; Excel, and many other spreadsheets, incorporate this option. Once the data has been input using either method, the data will be displayed in the data-box section of the main window. Fig. 1 shows the data-box containing a data set for the thermal conductivity of ammonia.

3.2. Degree of the rational function

The `Padé[N/M]` field allows the user to determine the degree in the polynomials (numerator and denominator). When zero is entered in the denominator the software calculates the polynomial approximation that best fits the data set, otherwise a rational approximation is generated; the least squares error method is used for finding the fitting parameters; see the algorithm in former section.

3.3. Buttons section

The buttons section contains seven buttons that perform different tasks. The `Confirm Data` button is activated only

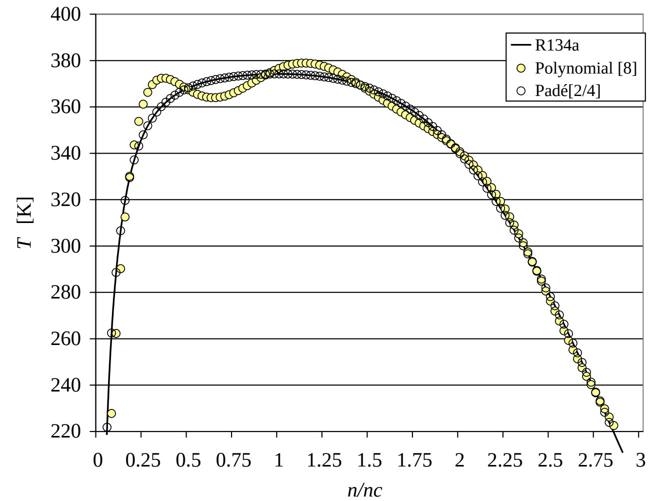

Fig. 4. Polynomial approximation vs. rational approximation in estimating the saturation temperature of R134a as a function of the density (n); n_c is the critical density; see [2].

when data is entered through the data field, its main function is to prevent the user from entering the wrong data. The `Coefficients` button re-activates the *results window* in the screen; in some cases the user, accidentally or in purpose, has closed the *results window* and he or she may want it back into the screen, for example, when the *matrix window* is displayed the *results window* is automatically closed.

The `Calculate` button, perhaps the most important button, calculates the rational approximation and displays the resulting approximation in the *results window*. Besides the coefficients (fitting parameters) the software calculates valuable information, useful to determine the goodness of the fit. The statistics calculated are based on the following

Table 2
Thermodynamic efficiency and EMF for a fuel cell operated with pure hydrogen

Temperature (K)	$\Delta_f G^\circ$ (kJ/mole)	EMF (V)	$\eta_{thermal}$ (%)
298.15	−228.5298	1.18	94.49
373.15	−225.0320	1.16	93.05
573.15	−215.2774	1.11	89.01
773.15	−204.9616	1.06	84.75
973.15	−194.1746	1.00	80.29
1173.15	−183.0214	0.95	75.68
1473.15	−165.8635	0.86	68.58

Table 1
Thermophysical properties for water (H_2O)

	$[N/M]$						R^2
C_p	[2/2]	33.253760	−0.007235433	3.047110E−05	−0.0001375154	5.058140E−07	0.9999
S°	[1/3]	119.670700	1.058446000	0.0045406960	−5.492381E−07	7.037198E−11	0.9999
$\Delta_f H^\circ$	[2/1]	−238.039200	−0.073690040	2.072838E−06	0.0002495145		0.9995
$\Delta_f G^\circ$	[1/2]	−241.365800	0.044332430	−1.770163E−05	4.030592E−08		0.9999
μ	[1/2]	−1.043642	0.031849010	−0.0003785168	1.976538E−07		0.9999
λ	[2/1]	31.182260	−0.111481900	0.0004250616	0.0025513490		0.9999

equations:

$$SSX = \sum_{i=1}^{k} (x_i - \bar{x})^2$$

$$SSE = \sum_{i=1}^{k} (y_i - R_i(x))^2$$

$$SST = \sum_{i=1}^{k} (y_i - \bar{y})^2$$

$$s^2 = \frac{SSE}{k - (N + M + 1)}$$

$$RMSE = s = (s^2)^{1/2}$$

$$R^2 = 1 - \frac{SSE}{SST}$$

$$R^2\,\text{Adj} = 1 - \frac{SSE(k-1)}{SST((k - (N + M + 1)) - 1)}$$

$$AAD = \frac{1}{k} \sum_{i=1}^{k} \frac{|R_i(x) - y_i|}{y_i} \times 100$$

The student distribution (`tstd` $\equiv t^*$) is reported for a 90% confidence interval. The student distribution is useful for calculating the confidence intervals for the coefficients; ($a_i \pm t^* \times sa_i$, $b_i \pm t^* \times sb_i$). The standard deviation for the coefficients can be determine from the diagonal elements in the covariance matrix (see `Matrices` button).

Table 3
Isobaric heat capacity (C_p, (J/(K mole)) for important fluids in SOFCs

T (K)	CH_4	C_2H_6	C_3H_8	CH_3OH	C_2H_5OH	CO_2	CO	H_2	H_2O	O_2	N_2	NH_3
243	33.9949	44.9101	61.8016	39.7383	57.0218	34.3148	29.0911	28.1892	33.4134	29.1888	29.0427	34.5178
273	34.8347	48.9953	68.2445	41.9984	61.6922	35.8628	29.0938	28.4581	33.5442	29.3633	29.0595	35.2962
303	35.9209	53.0443	74.5924	44.3234	66.4047	37.3021	29.1181	28.6794	33.6982	29.5476	29.0919	36.1106
333	37.2045	57.0437	80.8167	46.6911	71.0961	38.6426	29.1648	28.8575	33.8745	29.7421	29.1400	36.9561
363	38.6429	60.9821	86.8949	49.0817	75.7199	39.8933	29.2338	28.9977	34.0723	29.9471	29.2036	37.8277
393	40.1993	64.8496	92.8099	51.4777	80.2421	41.0617	29.3249	29.1056	34.2908	30.1627	29.2824	38.7209
423	41.8425	68.6376	98.5490	53.8642	84.6392	42.1550	29.4373	29.1869	34.5288	30.3890	29.3760	39.6313
453	43.5463	72.3393	104.1037	56.2283	88.8955	43.1793	29.5696	29.2471	34.7854	30.6254	29.4836	40.5547
483	45.2885	75.9492	109.4687	58.5595	93.0014	44.1401	29.7202	29.2914	35.0592	30.8713	29.6045	41.4872
513	47.0509	79.4628	114.6412	60.8488	96.9517	45.0424	29.8873	29.3247	35.3493	31.1258	29.7378	42.4254
543	48.8186	82.8770	119.6209	63.0894	100.7448	45.8908	30.0687	29.3510	35.6542	31.3875	29.8823	43.3659
573	50.5794	86.1895	124.4092	65.2756	104.3816	46.6893	30.2621	29.3738	35.9728	31.6548	30.0368	44.3059
603	52.3234	89.3990	129.0090	67.4032	107.8648	47.4415	30.4651	29.3961	36.3038	31.9257	30.2003	45.2426
633	54.0427	92.5047	133.4240	69.4693	111.1983	48.1508	30.6753	29.4203	36.6459	32.1980	30.3713	46.1736
663	55.7313	95.5068	137.6591	71.4718	114.3871	48.8203	30.8907	29.4482	36.9979	32.4696	30.5487	47.0968
693	57.3844	98.4059	141.7196	73.4094	117.4366	49.4527	31.1090	29.4812	37.3585	32.7381	30.7312	48.0104
723	58.9984	101.2030	145.6114	75.2817	120.3525	50.0505	31.3283	29.5202	37.7265	33.0012	30.9175	48.9126
753	60.5707	103.8998	149.3405	77.0888	123.1408	50.6161	31.5470	29.5660	38.1008	33.2570	31.1065	49.8020
783	62.0995	106.4981	152.9132	78.8311	125.8075	51.1515	31.7635	29.6188	38.4802	33.5035	31.2971	50.6776
813	63.5837	109.0000	156.3359	80.5097	128.3585	51.6588	31.9767	29.6788	38.8636	33.7393	31.4882	51.5381
843	65.0225	111.4078	159.6147	82.1257	130.7995	52.1396	32.1855	29.7460	39.2500	33.9633	31.6789	52.3829
873	66.4158	113.7241	162.7561	83.6807	133.1361	52.5958	32.3890	29.8203	39.6384	34.1748	31.8683	53.2111
903	67.7637	115.9515	165.7661	85.1763	135.3738	53.0287	32.5866	29.9012	40.0278	34.3732	32.0557	54.0223
933	69.0667	118.0928	168.6507	86.6143	137.5176	53.4398	32.7779	29.9886	40.4175	34.5587	32.2404	54.8161
963	70.3254	120.1508	171.4156	87.9966	139.5724	53.8304	32.9625	30.0819	40.8065	34.7315	32.4218	55.5920
993	71.5407	122.1282	174.0666	89.3250	141.5430	54.2017	33.1402	30.1809	41.1942	34.8920	32.5993	56.3501
1023	72.7133	124.0280	176.6090	90.6017	143.4337	54.5549	33.3110	30.2849	41.5799	35.0410	32.7727	57.0900
1053	73.8444	125.8530	179.0479	91.8285	145.2488	54.8909	33.4748	30.3936	41.9629	35.1793	32.9416	57.8119
1083	74.9352	127.6059	181.3883	93.0075	146.9922	55.2108	33.6318	30.5065	42.3427	35.3078	33.1057	58.5158
1113	75.9866	129.2895	183.6350	94.1405	148.6675	55.5155	33.7820	30.6231	42.7187	35.4274	33.2647	59.2017
1143	76.9999	130.9065	185.7924	95.2294	150.2784	55.8057	33.9257	30.7431	43.0905	35.5392	33.4187	59.8699
1173	77.9764	132.4596	187.8649	96.2762	151.8281	56.0823	34.0631	30.8659	43.4577	35.6439	33.5675	60.5205
1203	78.9171	133.9513	189.8565	97.2826	153.3198	56.3461	34.1943	30.9912	43.8198	35.7426	33.7110	61.1539
1233	79.8233	135.3842	191.7711	98.2504	154.7564	56.5976	34.3197	31.1186	44.1767	35.8360	33.8492	61.7701
1263	80.6962	136.7606	193.6125	99.1812	156.1405	56.8376	34.4394	31.2478	44.5279	35.9249	33.9823	62.3697
1293	81.5369	138.0829	195.3841	100.0767	157.4750	57.0666	34.5539	31.3783	44.8733	36.0100	34.1101	62.9529
1323	82.3466	139.3534	197.0892	100.9385	158.7621	57.2853	34.6633	31.5099	45.2127	36.0919	34.2329	63.5200
1353	83.1263	140.5743	198.7310	101.7680	160.0042	57.4941	34.7678	31.6422	45.5459	36.1711	34.3507	64.0714
1383	83.8771	141.7477	200.3124	102.5667	161.2035	57.6936	34.8679	31.7750	45.8728	36.2483	34.4637	64.6074
1413	84.6001	142.8755	201.8364	103.3359	162.3620	57.8842	34.9636	31.9080	46.1933	36.3237	34.5720	65.1285
1443	85.2963	143.9598	203.3055	104.0771	163.4816	58.0664	35.0553	32.0409	46.5072	36.3978	34.6756	65.6351
1473	85.9666	145.0024	204.7223	104.7913	164.5641	58.2406	35.1432	32.1735	46.8147	36.4708	34.7748	66.1274

The `Remove Row` button removes the last data added to data-box.

The `Matrices` button displays the matrices created in the generation of the Padé correlations (see Fig. 2). The results are presented in the *Matrices window*. The reason we keep them available is because they are useful to find errors or for checking how the approximation is working.

The `Delete` button deletes everything and leaves the environment ready for a new approximation.

The `Plot Results` button plots the data set, the estimated values (approximation) and the residual plot, in two additional windows. This is the first analysis that is recommended to see the goodness of the fit. A visual inspection is useful for identifying the randomness of the errors and also to check the convergence of the approximation. When the approximation does not converge a truncated plot is shown. When the approximation does converge the software evaluates around 5000 points between: 160% of the highest independent value (x_{max}), and −160% of the lowest independent value (x_{min}). This allows the user to see if the approximation preserves a *reasonable* trend, hence can be used for extrapolation purposes (see Fig. 3).

4. Examples

The **Padé** software was used in [1] for calculating thermophysical properties of fluids common to SOFCs. The reason why rational functions are considered in [1] is because they are useful when few experimental data points are

Table 4
Entropy of formation ($\Delta_f S^\circ$, (J/(K mole)) for important fluids in SOFCs

T (K)	CH_4	C_2H_6	C_3H_8	CH_3OH	C_2H_5OH	CO_2	CO	H_2	H_2O	O_2	N_2	NH_3
243	179.1128	219.4431	256.3626	231.9127	269.2160	206.4265	191.5435	124.8743	181.8915	199.1856	185.6099	185.4343
273	182.8172	224.7565	263.9572	236.2946	275.9874	210.4144	194.9809	128.1440	185.7302	202.3573	189.0169	189.3704
303	186.3773	229.9864	271.4395	240.5673	282.6136	214.1865	198.0660	131.1154	189.2183	205.3060	192.0702	193.0441
333	189.8072	235.1348	278.8109	244.7357	289.0994	217.7631	200.8623	133.8334	192.4133	208.0573	194.8354	196.4914
363	193.1191	240.2031	286.0733	248.8044	295.4496	221.1624	203.4188	136.3343	195.3605	210.6329	197.3627	199.7417
393	196.3240	245.1932	293.2282	252.7779	301.6687	224.3999	205.7738	138.6477	198.0964	213.0514	199.6908	202.8197
423	199.4311	250.1067	300.2772	256.6602	307.7612	227.4896	207.9578	140.7979	200.6507	215.3289	201.8504	205.7460
453	202.4489	254.9450	307.2219	260.4552	313.7310	230.4439	209.9954	142.8052	203.0477	217.4793	203.8660	208.5381
483	205.3848	259.7097	314.0638	264.1667	319.5821	233.2737	211.9064	144.6867	205.3073	219.5148	205.7572	211.2107
513	208.2452	264.4023	320.8044	267.7982	325.3185	235.9888	213.7072	146.4568	207.4464	221.4462	207.5402	213.7765
543	211.0360	269.0242	327.4453	271.3529	330.9436	238.5979	215.4113	148.1277	209.4791	223.2827	209.2283	216.2463
573	213.7624	273.5769	333.9878	274.8339	336.4610	241.1090	217.0302	149.7099	211.4172	225.0327	210.8327	218.6295
603	216.4291	278.0616	340.4335	278.2443	341.8741	243.5290	218.5733	151.2123	213.2708	226.7036	212.3625	220.9344
633	219.0402	282.4798	346.7838	281.5867	347.1859	245.8645	220.0487	152.6429	215.0488	228.3018	213.8256	223.1679
663	221.5994	286.8328	353.0400	284.8640	352.3996	248.1211	221.4633	154.0084	216.7587	229.8332	215.2288	225.3364
693	224.1101	291.1217	359.2035	288.0787	357.5182	250.3040	222.8230	155.3148	218.4068	231.3031	216.5776	227.4452
723	226.5752	295.3478	365.2758	291.2331	362.5444	252.4182	224.1329	156.5672	219.9989	232.7161	217.8772	229.4993
753	228.9975	299.5124	371.2581	294.3295	367.4810	254.4678	225.3975	157.7703	221.5399	234.0766	219.1317	231.5027
783	231.3794	303.6166	377.1517	297.3702	372.3307	256.4568	226.6205	158.9282	223.0342	235.3882	220.3449	233.4594
813	233.7231	307.6615	382.9580	300.3572	377.0958	258.3889	227.8053	160.0445	224.4855	236.6545	221.5200	235.3727
843	236.0307	311.6482	388.6782	303.2924	381.7789	260.2673	228.9549	161.1225	225.8973	237.8786	222.6598	237.2455
873	238.3037	315.5778	394.3135	306.1779	386.3822	262.0951	230.0719	162.1649	227.2725	239.0634	223.7670	239.0804
903	240.5440	319.4515	399.8653	309.0153	390.9081	263.8751	231.1585	163.1745	228.6138	240.2114	224.8436	240.8800
933	242.7529	323.2701	405.3346	311.8065	395.3586	265.6099	232.2167	164.1535	229.9235	241.3251	225.8917	242.6462
963	244.9318	327.0348	410.7228	314.5530	399.7358	267.3018	233.2484	165.1040	231.2039	242.4066	226.9130	244.3811
993	247.0817	330.7464	416.0309	317.2564	404.0418	268.9530	234.2552	166.0280	232.4567	243.4579	227.9092	246.0862
1023	249.2039	334.4061	421.2602	319.9183	408.2784	270.5655	235.2384	166.9272	233.6837	244.4809	228.8816	247.7632
1053	251.2991	338.0146	426.4117	322.5400	412.4476	272.1412	236.1994	167.8032	234.8863	245.4773	229.8316	249.4134
1083	253.3683	341.5729	431.4867	325.1230	416.5511	273.6818	237.1393	168.6573	236.0661	246.4485	230.7602	251.0381
1113	255.4122	345.0819	436.4861	327.6685	420.5907	275.1890	238.0592	169.4910	237.2242	247.3962	231.6685	252.6384
1143	257.4315	348.5425	441.4112	330.1779	424.5679	276.6641	238.9599	170.3053	238.3618	248.3215	232.5574	254.2153
1173	259.4268	351.9555	446.2629	332.6523	428.4845	278.1087	239.8423	171.1015	239.4799	249.2257	233.4278	255.7697
1203	261.3986	355.3217	451.0423	335.0929	432.3420	279.5240	240.7071	171.8805	240.5793	250.1099	234.2806	257.3024
1233	263.3473	358.6420	455.7504	337.5008	436.1419	280.9112	241.5550	172.6432	241.6610	250.9753	235.1163	258.8141
1263	265.2734	361.9171	460.3883	339.8770	439.8857	282.2715	242.3867	173.3905	242.7258	251.8228	235.9356	260.3056
1293	267.1772	365.1479	464.9570	342.2227	443.5747	283.6058	243.2027	174.1232	243.7742	252.6534	236.7392	261.7773
1323	269.0589	368.3350	469.4574	344.5388	447.2103	284.9152	244.0034	174.8420	244.8069	253.4678	237.5275	263.2299
1353	270.9189	371.4792	473.8905	346.8262	450.7939	286.2005	244.7894	175.5476	245.8246	254.2669	238.3012	264.6637
1383	272.7574	374.5813	478.2574	349.0858	454.3266	287.4627	245.5610	176.2407	246.8277	255.0515	239.0605	266.0793
1413	274.5743	377.6419	482.5588	351.3186	457.8099	288.7025	246.3186	176.9218	247.8167	255.8222	239.8061	267.4769
1443	276.3700	380.6618	486.7959	353.5253	461.2447	289.9207	247.0626	177.5914	248.7921	256.5797	240.5383	268.8570
1473	278.1445	383.6416	490.9694	355.7069	464.6323	291.1180	247.7932	178.2502	249.7541	257.3246	241.2573	270.2197

available and when polynomial approximation can not be used for extrapolation. Two examples are reported in [1] showing these qualities. Here a different situation is presented. Another very important feature of rational functions is that they are able to represent complicated structures. For complicated we mean functions that do not preserve a *smooth* tendency.

4.1. Example 1

The saturation temperature for the refrigerant R134a is approximated using both, rational and polynomial approximation. The data set was taken from [2]; Ray et al. [2] report the method of rational approximation in the generation of equations of state that are simpler than the ones found in the literature for real fluids. The **Padé** software was used for this purpose, the data set was generated from correlations reported in [2]. The results clearly show (see Fig. 4) the inability of the polynomial to approximate the data specially in the top of the curve. Rational approximation works better when the shape of the function being approximated change suddenly, as in this case, where after an almost constant trend (top) the function suddenly starts to decrease.

4.2. Example 2: efficiency of a fuel cell

The theoretical maximum fuel cell efficiency (η_{thermal}) for burning hydrogen can be readily determined from the thermophysical properties reported in [1]. Lets assume that the thermodynamic efficiency is required for a fuel cell fueled

Table 5
Enthalpy of formation ($\Delta_f H^\circ$, (kJ/mole)) for important fluids in SOFCs

T (K)	CH_4	C_2H_6	C_3H_8	CH_3OH	C_2H_5OH	CO_2	CO	H_2	H_2O	O_2	N_2	NH_3
243	−73.2359	−80.9368	−99.7372	−198.6534	−231.6243	−393.4457	−110.8378	0.0000	−241.1991	0.0000	0.0000	−44.7058
273	−74.1145	−82.6278	−102.0141	−199.9374	−233.3840	−393.4588	−110.6292	0.0000	−241.5484	0.0000	0.0000	−45.4012
303	−75.0130	−84.2503	−104.1724	−201.1582	−235.0522	−393.4763	−110.4597	0.0000	−241.8894	0.0000	0.0000	−46.0711
333	−75.9213	−85.8047	−106.2159	−202.3187	−236.6319	−393.4978	−110.3254	0.0000	−242.2223	0.0000	0.0000	−46.7154
363	−76.8301	−87.2912	−108.1485	−203.4216	−238.1263	−393.5232	−110.2225	0.0000	−242.5471	0.0000	0.0000	−47.3342
393	−77.7317	−88.7106	−109.9741	−204.4695	−239.5381	−393.5521	−110.1479	0.0000	−242.8642	0.0000	0.0000	−47.9274
423	−78.6191	−90.0636	−111.6964	−205.4647	−240.8705	−393.5845	−110.0988	0.0000	−243.1735	0.0000	0.0000	−48.4953
453	−79.4869	−91.3511	−113.3192	−206.4096	−242.1262	−393.6199	−110.0728	0.0000	−243.4754	0.0000	0.0000	−49.0380
483	−80.3303	−92.5744	−114.8462	−207.3063	−243.3082	−393.6584	−110.0677	0.0000	−243.7699	0.0000	0.0000	−49.5558
513	−81.1458	−93.7346	−116.2809	−208.1570	−244.4193	−393.6995	−110.0816	0.0000	−244.0571	0.0000	0.0000	−50.0491
543	−81.9306	−94.8331	−117.6269	−208.9635	−245.4623	−393.7432	−110.1127	0.0000	−244.3373	0.0000	0.0000	−50.5181
573	−82.6828	−95.8715	−118.8877	−209.7278	−246.4397	−393.7893	−110.1597	0.0000	−244.6106	0.0000	0.0000	−50.9632
603	−83.4012	−96.8512	−120.0665	−210.4515	−247.3544	−393.8376	−110.2211	0.0000	−244.8771	0.0000	0.0000	−51.3850
633	−84.0849	−97.7739	−121.1667	−211.1365	−248.2087	−393.8878	−110.2956	0.0000	−245.1369	0.0000	0.0000	−51.7839
663	−84.7338	−98.6413	−122.1915	−211.7841	−249.0054	−393.9399	−110.3823	0.0000	−245.3901	0.0000	0.0000	−52.1604
693	−85.3481	−99.4551	−123.1439	−212.3961	−249.7468	−393.9937	−110.4800	0.0000	−245.6370	0.0000	0.0000	−52.5150
723	−85.9281	−100.2170	−124.0270	−212.9738	−250.4353	−394.0490	−110.5879	0.0000	−245.8775	0.0000	0.0000	−52.8483
753	−86.4747	−100.9288	−124.8437	−213.5186	−251.0732	−394.1057	−110.7051	0.0000	−246.1119	0.0000	0.0000	−53.1608
783	−86.9887	−101.5924	−125.5968	−214.0317	−251.6627	−394.1636	−110.8310	0.0000	−246.3402	0.0000	0.0000	−53.4532
813	−87.4711	−102.2094	−126.2889	−214.5146	−252.2062	−394.2227	−110.9649	0.0000	−246.5626	0.0000	0.0000	−53.7261
843	−87.9233	−102.7817	−126.9229	−214.9682	−252.7056	−394.2827	−111.1060	0.0000	−246.7791	0.0000	0.0000	−53.9799
873	−88.3463	−103.3110	−127.5011	−215.3939	−253.1630	−394.3436	−111.2539	0.0000	−246.9900	0.0000	0.0000	−54.2155
903	−88.7414	−103.7990	−128.0261	−215.7926	−253.5805	−394.4052	−111.4080	0.0000	−247.1952	0.0000	0.0000	−54.4332
933	−89.1100	−104.2475	−128.5003	−216.1654	−253.9599	−394.4674	−111.5679	0.0000	−247.3948	0.0000	0.0000	−54.6339
963	−89.4533	−104.6581	−128.9258	−216.5133	−254.3031	−394.5303	−111.7331	0.0000	−247.5891	0.0000	0.0000	−54.8180
993	−89.7726	−105.0326	−129.3050	−216.8372	−254.6118	−394.5935	−111.9032	0.0000	−247.7780	0.0000	0.0000	−54.9862
1023	−90.0691	−105.3724	−129.6398	−217.1381	−254.8879	−394.6571	−112.0778	0.0000	−247.9618	0.0000	0.0000	−55.1391
1053	−90.3440	−105.6792	−129.9325	−217.4168	−255.1330	−394.7210	−112.2566	0.0000	−248.1403	0.0000	0.0000	−55.2773
1083	−90.5985	−105.9545	−130.1848	−217.6741	−255.3486	−394.7851	−112.4392	0.0000	−248.3139	0.0000	0.0000	−55.4013
1113	−90.8337	−106.1997	−130.3988	−217.9108	−255.5364	−394.8494	−112.6254	0.0000	−248.4825	0.0000	0.0000	−55.5117
1143	−91.0507	−106.4164	−130.5761	−218.1278	−255.6979	−394.9137	−112.8149	0.0000	−248.6462	0.0000	0.0000	−55.6091
1173	−91.2505	−106.6059	−130.7186	−218.3256	−255.8344	−394.9781	−113.0074	0.0000	−248.8051	0.0000	0.0000	−55.6941
1203	−91.4340	−106.7695	−130.8279	−218.5050	−255.9474	−395.0425	−113.2027	0.0000	−248.9594	0.0000	0.0000	−55.7671
1233	−91.6023	−106.9086	−130.9056	−218.6667	−256.0383	−395.1069	−113.4005	0.0000	−249.1090	0.0000	0.0000	−55.8287
1263	−91.7562	−107.0243	−130.9531	−218.8114	−256.1082	−395.1711	−113.6006	0.0000	−249.2541	0.0000	0.0000	−55.8794
1293	−91.8965	−107.1180	−130.9721	−218.9395	−256.1584	−395.2353	−113.8030	0.0000	−249.3947	0.0000	0.0000	−55.9197
1323	−92.0239	−107.1907	−130.9638	−219.0518	−256.1901	−395.2993	−114.0073	0.0000	−249.5309	0.0000	0.0000	−55.9501
1353	−92.1393	−107.2435	−130.9297	−219.1488	−256.2045	−395.3633	−114.2133	0.0000	−249.6628	0.0000	0.0000	−55.9710
1383	−92.2434	−107.2776	−130.8710	−219.2311	−256.2026	−395.4271	−114.4210	0.0000	−249.7905	0.0000	0.0000	−55.9829
1413	−92.3367	−107.2939	−130.7889	−219.2990	−256.1855	−395.4908	−114.6302	0.0000	−249.9140	0.0000	0.0000	−55.9862
1443	−92.4199	−107.2934	−130.6847	−219.3533	−256.1543	−395.5543	−114.8408	0.0000	−250.0334	0.0000	0.0000	−55.9814
1473	−92.4936	−107.2770	−130.5594	−219.3943	−256.1098	−395.6178	−115.0525	0.0000	−250.1487	0.0000	0.0000	−55.9689

with pure hydrogen. The burning of hydrogen takes place under the following conditions:

$$H_2 + \tfrac{1}{2}O_2 \rightarrow H_2O_g$$

$$\eta_{thermal}(\%) = \frac{\Delta_f G^\circ(T)}{\Delta_f H_{Tr}{}^\circ} \times 100$$

$$Tr = 298.15\,K$$

$$\Delta_f H_{Tr}{}^\circ = -241.8349\,kJ/mole^*$$

The value for $\Delta_f H_{Tr}{}^\circ$ is calculated using the correlation reported in Table 1 ($\Delta_f H^\circ$).

The open circuit voltage (EMF) can be also determined directly from the correlations for the Gibbs free energy of formation reported in the paper. The EMF is defined as:

$$EMF = \frac{-\Delta_f G^\circ(T)}{2F}$$

$$F = 96,485\,C$$

Using the former equations and the correlation reported in Table 1 ($\Delta_f G^\circ$), we can investigate the maximum voltage obtainable from the cell and the thermodynamic limit in the cell. The results are shown in Table 2.

Similar results can be obtained for different reactions, using the appropriate thermodynamic relations; this example was taken from [3], but the results where calculated with the thermophysical properties reported in Table 1.

Table 6
Gibbs Free Energy of formation ($\Delta_f G^\circ$, (kJ/mole)) for important fluids in SOFCs

T (K)	CH_4	C_2H_6	C_3H_8	CH_3OH	C_2H_5OH	CO_2	CO	H_2	H_2O	O_2	N_2	NH_3
243	−55.0876	−41.6849	−38.2433	−169.4671	−179.9828	−394.2239	−132.2741	0.0000	−231.0370	0.0000	0.0000	−21.7488
273	−52.7698	−36.4884	−30.2798	−165.6139	−173.4740	−394.3178	−134.9763	0.0000	−229.6830	0.0000	0.0000	−18.8397
303	−50.3594	−31.1858	−22.1534	−161.6787	−166.7876	−394.4092	−137.6802	0.0000	−228.3128	0.0000	0.0000	−15.8655
333	−47.8639	−25.7813	−13.8751	−157.6656	−159.9467	−394.4979	−140.3855	0.0000	−226.9265	0.0000	0.0000	−12.8334
363	−45.2900	−20.2796	−5.4553	−153.5785	−152.9710	−394.5840	−143.0920	0.0000	−225.5245	0.0000	0.0000	−9.7497
393	−42.6444	−14.6854	3.0956	−149.4215	−145.8772	−394.6677	−145.7993	0.0000	−224.1071	0.0000	0.0000	−6.6197
423	−39.9329	−9.0035	11.7677	−145.1986	−138.6797	−394.7489	−148.5072	0.0000	−222.6746	0.0000	0.0000	−3.4481
453	−37.1613	−3.2388	20.5513	−140.9137	−131.3910	−394.8276	−151.2154	0.0000	−221.2274	0.0000	0.0000	−0.2393
483	−34.3346	2.6038	29.4373	−136.5710	−124.0216	−394.9039	−153.9236	0.0000	−219.7658	0.0000	0.0000	3.0031
513	−31.4577	8.5192	38.4168	−132.1741	−116.5810	−394.9779	−156.6313	0.0000	−218.2901	0.0000	0.0000	6.2758
543	−28.5350	14.5025	47.4814	−127.7271	−109.0772	−395.0495	−159.3384	0.0000	−216.8007	0.0000	0.0000	9.5759
573	−25.5704	20.5488	56.6232	−123.2337	−101.5175	−395.1188	−162.0444	0.0000	−215.2979	0.0000	0.0000	12.9008
603	−22.5678	26.6530	65.8345	−118.6975	−93.9080	−395.1859	−164.7491	0.0000	−213.7822	0.0000	0.0000	16.2480
633	−19.5304	32.8104	75.1082	−114.1222	−86.2543	−395.2508	−167.4520	0.0000	−212.2538	0.0000	0.0000	19.6156
663	−16.4615	39.0163	84.4377	−109.5110	−78.5613	−395.3134	−170.1528	0.0000	−210.7131	0.0000	0.0000	23.0015
693	−13.3638	45.2660	93.8167	−104.8675	−70.8334	−395.3739	−172.8513	0.0000	−209.1606	0.0000	0.0000	26.4042
723	−10.2401	51.5551	103.2393	−100.1946	−63.0744	−395.4323	−175.5469	0.0000	−207.5965	0.0000	0.0000	29.8219
753	−7.0926	57.8793	112.7001	−95.4955	−55.2878	−395.4886	−178.2396	0.0000	−206.0212	0.0000	0.0000	33.2534
783	−3.9237	64.2345	122.1942	−90.7729	−47.4766	−395.5428	−180.9289	0.0000	−204.4352	0.0000	0.0000	36.6973
813	−0.7351	70.6169	131.7170	−86.0297	−39.6436	−395.5950	−183.6145	0.0000	−202.8389	0.0000	0.0000	40.1524
843	2.4712	77.0226	141.2643	−81.2682	−31.7913	−395.6452	−186.2962	0.0000	−201.2325	0.0000	0.0000	43.6177
873	5.6935	83.4485	150.8324	−76.4908	−23.9219	−395.6934	−188.9737	0.0000	−199.6165	0.0000	0.0000	47.0922
903	8.9304	89.8912	160.4179	−71.6997	−16.0374	−395.7397	−191.6467	0.0000	−197.9913	0.0000	0.0000	50.5750
933	12.1804	96.3480	170.0178	−66.8969	−8.1396	−395.7841	−194.3151	0.0000	−196.3572	0.0000	0.0000	54.0653
963	15.4424	102.8161	179.6294	−62.0840	−0.2301	−395.8266	−196.9787	0.0000	−194.7148	0.0000	0.0000	57.5623
993	18.7151	109.2934	189.2504	−57.2627	7.6896	−395.8672	−199.6372	0.0000	−193.0643	0.0000	0.0000	61.0653
1023	21.9975	115.7778	198.8788	−52.4343	15.6182	−395.9060	−202.2905	0.0000	−191.4061	0.0000	0.0000	64.5737
1053	25.2886	122.2675	208.5130	−47.6000	23.5544	−395.9431	−204.9385	0.0000	−189.7407	0.0000	0.0000	68.0869
1083	28.5877	128.7613	218.1517	−42.7608	31.4973	−395.9783	−207.5812	0.0000	−188.0684	0.0000	0.0000	71.6042
1113	31.8937	135.2581	227.7937	−37.9175	39.4458	−396.0118	−210.2183	0.0000	−186.3897	0.0000	0.0000	75.1253
1143	35.2062	141.7570	237.4384	−33.0705	47.3991	−396.0435	−212.8499	0.0000	−184.7048	0.0000	0.0000	78.6497
1173	38.5243	148.2579	247.0852	−28.2203	55.3563	−396.0736	−215.4760	0.0000	−183.0143	0.0000	0.0000	82.1768
1203	41.8474	154.7605	256.7339	−23.3670	63.3167	−396.1020	−218.0964	0.0000	−181.3186	0.0000	0.0000	85.7063
1233	45.1751	161.2652	266.3846	−18.5105	71.2797	−396.1288	−220.7114	0.0000	−179.6179	0.0000	0.0000	89.2378
1263	48.5068	167.7725	276.0374	−13.6507	79.2447	−396.1539	−223.3208	0.0000	−177.9127	0.0000	0.0000	92.7709
1293	51.8420	174.2834	285.6928	−8.7869	87.2111	−396.1774	−225.9248	0.0000	−176.2034	0.0000	0.0000	96.3053
1323	55.1804	180.7993	295.3516	−3.9186	95.1785	−396.1994	−228.5234	0.0000	−174.4904	0.0000	0.0000	99.8408
1353	58.5215	187.3216	305.0147	0.9552	103.1464	−396.2198	−231.1167	0.0000	−172.7740	0.0000	0.0000	103.3769
1383	61.8649	193.8525	314.6830	5.8355	111.1145	−396.2387	−233.7048	0.0000	−171.0546	0.0000	0.0000	106.9135
1413	65.2104	200.3942	324.3580	10.7237	119.0823	−396.2560	−236.2879	0.0000	−169.3327	0.0000	0.0000	110.4503
1443	68.5577	206.9494	334.0410	15.6213	127.0496	−396.2719	−238.8660	0.0000	−167.6085	0.0000	0.0000	113.9871
1473	71.9065	213.5212	343.7337	20.5301	135.0162	−396.2863	−241.4394	0.0000	−165.8825	0.0000	0.0000	117.5235

Table 7
Enthalpy (H°, (kJ/mole)) for important fluids in SOFCs

T (K)	CH_4	C_2H_6	C_3H_8	CH_3OH	C_2H_5OH	CO_2	CO	H_2	H_2O	O_2	N_2	NH_3
243	−76.7995	−86.7074	−107.6363	−203.1974	−238.1428	−395.5232	−112.1626		−243.7305			−47.8128
273	−75.7638	−85.2881	−105.6561	−202.0386	−236.3918	−394.4509	−111.2706		−242.7045			−46.7831
303	−74.7002	−83.7509	−103.4956	−200.7885	−234.4852	−393.3401	−110.3866		−241.6788			−45.7262
333	−73.6020	−82.0965	−101.1558	−199.4511	−232.4281	−392.1927	−109.5074		−240.6522			−44.6415
363	−72.4639	−80.3260	−98.6385	−198.0297	−230.2260	−391.0103	−108.6303		−239.6235			−43.5283
393	−71.2816	−78.4406	−95.9462	−196.5274	−227.8840	−389.7947	−107.7531		−238.5918			−42.3864
423	−70.0521	−76.4420	−93.0821	−194.9471	−225.4072	−388.5474	−106.8739		−237.5559			−41.2153
453	−68.7729	−74.3319	−90.0498	−193.2917	−222.8007	−387.2700	−105.9913		−236.5148			−40.0150
483	−67.4423	−72.1126	−86.8537	−191.5636	−220.0694	−385.9639	−105.1042		−235.4675			−38.7853
513	−66.0594	−69.7864	−83.4984	−189.7654	−217.2181	−384.6305	−104.2117		−234.4133			−37.5262
543	−64.6236	−67.3557	−79.9889	−187.8993	−214.2516	−383.2711	−103.3131		−233.3511			−36.2380
573	−63.1347	−64.8234	−76.3307	−185.9675	−211.1745	−381.8869	−102.4081		−232.2804			−34.9206
603	−61.5929	−62.1923	−72.5293	−183.9722	−207.9913	−380.4793	−101.4962		−231.2004			−33.5745
633	−59.9987	−59.4654	−68.5905	−181.9153	−204.7062	−379.0493	−100.5774		−230.1105			−32.1999
663	−58.3529	−56.6457	−64.5201	−179.7988	−201.3236	−377.5980	−99.6517		−229.0101			−30.7972
693	−56.6564	−53.7363	−60.3238	−177.6246	−197.8475	−376.1266	−98.7191		−227.8987			−29.3668
723	−54.9103	−50.7405	−56.0074	−175.3945	−194.2819	−374.6360	−97.7799		−226.7761			−27.9092
753	−53.1158	−47.6614	−51.5765	−173.1104	−190.6305	−373.1272	−96.8341		−225.6418			−26.4249
783	−51.2743	−44.5023	−47.0364	−170.7738	−186.8971	−371.6011	−95.8822		−224.4955			−24.9144
813	−49.3871	−41.2661	−42.3924	−168.3865	−183.0851	−370.0587	−94.9243		−223.3372			−23.3783
843	−47.4558	−37.9561	−37.6494	−165.9502	−179.1979	−368.5008	−93.9608		−222.1665			−21.8171
873	−45.4817	−34.5753	−32.8118	−163.4664	−175.2388	−366.9282	−92.9919		−220.9835			−20.2314
903	−43.4665	−31.1265	−27.8840	−160.9367	−171.2109	−365.3417	−92.0180		−219.7882			−18.6217
933	−41.4115	−27.6126	−22.8698	−158.3627	−167.1170	−363.7420	−91.0394		−218.5805			−16.9885
963	−39.3183	−24.0364	−17.7729	−155.7459	−162.9600	−362.1300	−90.0563		−217.3605			−15.3323
993	−37.1883	−20.4004	−12.5964	−153.0879	−158.7427	−360.5062	−89.0690		−216.1283			−13.6538
1023	−35.0230	−16.7070	−7.3432	−150.3900	−154.4674	−358.8713	−88.0775		−214.8841			−11.9532
1053	−32.8237	−12.9587	−2.0161	−147.6538	−150.1367	−357.2261	−87.0821		−213.6281			−10.2312
1083	−30.5917	−9.1576	3.3828	−144.8807	−145.7528	−355.5710	−86.0829		−212.3604			−8.4882
1113	−28.3283	−5.3058	8.8513	−142.0722	−141.3178	−353.9068	−85.0798		−211.0812			−6.7245
1143	−26.0346	−1.4052	14.3873	−139.2296	−136.8337	−352.2339	−84.0727		−209.7910			−4.9406
1173	−23.7117	2.5423	19.9889	−136.3544	−132.3025	−350.5529	−83.0617		−208.4899			−3.1368
1203	−21.3606	6.5352	25.6544	−133.4479	−127.7259	−348.8643	−82.0464		−207.1781			−1.3137
1233	−18.9823	10.5719	31.3817	−130.5116	−123.1055	−347.1687	−81.0266		−205.8561			0.5286
1263	−16.5776	14.6508	37.1687	−127.5468	−118.4428	−345.4665	−80.0020		−204.5242			2.3894
1293	−14.1471	18.7707	43.0131	−124.5549	−113.7394	−343.7581	−78.9721		−203.1825			4.2685
1323	−11.6915	22.9302	48.9121	−121.5372	−108.9964	−342.0441	−77.9363		−201.8316			6.1653
1353	−9.2114	27.1282	54.8625	−118.4950	−104.2151	−340.3248	−76.8940		−200.4716			8.0793
1383	−6.7071	31.3635	60.8603	−115.4298	−99.3966	−338.6007	−75.8444		−199.1030			10.0100
1413	−4.1789	35.6349	66.9010	−112.3429	−94.5418	−336.8721	−74.7869		−197.7261			11.9565
1443	−1.6269	39.9414	72.9788	−109.2355	−89.6516	−335.1395	−73.7203		−196.3411			13.9183
1473	0.9487	44.2819	79.0873	−106.1089	−84.7268	−333.4031	−72.6438		−194.9485			15.8942

Table 8
Viscosity (μ, (μPa s)) for important fluids in SOFCs

T (K)	CH_4	C_2H_6	C_3H_8	CH_3OH	C_2H_5OH	CO_2	CO	H_2	H_2O	O_2	N_2	NH_3
243	9.3102	7.5520	6.9563	8.5015	7.8520	12.2185	15.2330	7.7968	7.2803	17.4632	15.2330	8.2250
273	10.3384	8.5212	7.6752	9.2765	8.4846	13.7106	16.7335	8.4080	8.3950	19.2312	16.7335	9.0712
303	11.3259	9.4574	8.3985	10.1063	9.1668	15.1740	18.1537	9.0063	9.5263	20.9150	18.1537	10.0754
333	12.2764	10.3630	9.1237	10.9877	9.8970	16.6073	19.5069	9.5925	10.6735	22.5257	19.5069	11.1087
363	13.1931	11.2402	9.8482	11.9154	10.6715	18.0094	20.8031	10.1674	11.8355	24.0723	20.8031	12.1541
393	14.0789	12.0909	10.5692	12.8814	11.4838	19.3799	22.0500	10.7315	13.0113	25.5622	22.0500	13.1989
423	14.9365	12.9171	11.2840	13.8756	12.3244	20.7187	23.2537	11.2855	14.1999	27.0015	23.2537	14.2336
453	15.7681	13.7203	11.9898	14.8853	13.1804	22.0260	24.4191	11.8300	15.3999	28.3955	24.4191	15.2514
483	16.5756	14.5022	12.6839	15.8962	14.0363	23.3022	25.5503	12.3654	16.6103	29.7486	25.5503	16.2474
513	17.3611	15.2639	13.3637	16.8931	14.8739	24.5478	26.6506	12.8922	17.8296	31.0645	26.6506	17.2183
543	18.1261	16.0069	14.0266	17.8609	15.6742	25.7637	27.7228	13.4110	19.0566	32.3466	27.7228	18.1617
573	18.8720	16.7322	14.6701	18.7860	16.4187	26.9507	28.7695	13.9220	20.2898	33.5976	28.7695	19.0763
603	19.6003	17.4410	15.2919	19.6576	17.0912	28.1096	29.7927	14.4257	21.5278	34.8200	29.7927	19.9614
633	20.3121	18.1341	15.8900	20.4685	17.6802	29.2415	30.7942	14.9224	22.7690	36.0160	30.7942	20.8168
663	21.0086	18.8127	16.4624	21.2164	18.1802	30.3472	31.7757	15.4126	24.0120	37.1876	31.7757	21.6427
693	21.6907	19.4773	17.0076	21.9041	18.5925	31.4277	32.7387	15.8965	25.2552	38.3364	32.7387	22.4395
723	22.3594	20.1289	17.5240	22.5395	18.9258	32.4842	33.6845	16.3743	26.4969	39.4641	33.6845	23.2077
753	23.0155	20.7682	18.0104	23.1356	19.1955	33.5174	34.6141	16.8465	27.7356	40.5719	34.6141	23.9483
783	23.6597	21.3957	18.4661	23.7101	19.4228	34.5285	35.5288	17.3132	28.9696	41.6611	35.5288	24.6620
813	24.2928	22.0122				35.5182	36.4294	17.7747	30.1973	42.7329	36.4294	25.3498

Table 8 (*Continued*)

T (K)	CH_4	C_2H_6	C_3H_8	CH_3OH	C_2H_5OH	CO_2	CO	H_2	H_2O	O_2	N_2	NH_3
843	24.9155	22.6182				36.4877	37.3169	18.2312	31.4170	43.7883	37.3169	26.0127
873	25.5283	23.2143				37.4378	38.1920	18.6829	32.6271	44.8283	38.1920	26.6515
903	26.1317	23.8009				38.3693	39.0556	19.1302	33.8261	45.8536	39.0556	27.2673
933	26.7263	24.3785				39.2831	39.9083	19.5730	35.0122	46.8652	39.9083	27.8611
963	27.3125	24.9476				40.1800	40.7508	20.0117	36.1840	47.8636	40.7508	28.4337
993	27.8908	25.5085				41.0608	41.5837	20.4464	37.3398	48.8497	41.5837	28.9861
1023	28.4616	26.0617				41.9263	42.4077	20.8772	38.4783	49.8241	42.4077	29.5192
1053	29.0253	26.6074				42.7771	43.2231	21.3043	39.5979	50.7872	43.2231	30.0338
1083	29.5822	27.1462				43.6141	44.0306	21.7280	40.6973	51.7398	44.0306	30.5307
1113	30.1325	27.6782				44.4378	44.8307	22.1482	41.7752	52.6823	44.8307	31.0108
1143	30.6768	28.2037				45.2489	45.6237	22.5651	42.8302	53.6151	45.6237	31.4747
1173	31.2151	28.7231				46.0480	46.4102	22.9790	43.8613	54.5388	46.4102	31.9232
1203	31.7478	29.2366				46.8358	47.1905	23.3897	44.8671	55.4538	47.1905	32.3569
1233	32.2752	29.7445				47.6128	47.9650	23.7976	45.8469	56.3604	47.9650	32.7766
1263	32.7974	30.2469				48.3795	48.7341	24.2027	46.7995	57.2591	48.7341	33.1827
1293	33.3147	30.7442				49.1364	49.4983	24.6051	47.7241	58.1502	49.4983	33.5760
1323	33.8273	31.2365				49.8842	50.2577	25.0048	48.6199	59.0340	50.2577	33.9570
1353	34.3354	31.7240				50.6232	51.0127	25.4021	49.4862	59.9110	51.0127	34.3261
1383	34.8391	32.2069				51.3539	51.7638	25.7969	50.3223	60.7813	51.7638	34.6840
1413	35.3387	32.6855				52.0767	52.5111	26.1894	51.1279	61.6454	52.5111	35.0310
1443	35.8342	33.1598				52.7922	53.2549	26.5797	51.9024	62.5034	53.2549	35.3676
1473	36.3259	33.6300				53.5006	53.9957	26.9677	52.6454	63.3557	53.9957	35.6944

Table 9

Thermal conductivity (λ, (mW/(m K)]) for important fluids in SOFCs

T (K)	CH_4	C_2H_6	C_3H_8	CH_3OH	C_2H_5OH	CO_2	CO	H_2	H_2O	O_2	N_2	NH_3
243	27.1140	14.9184	12.3481			12.3899	20.5623	154.2662		21.8598	21.8655	20.9854
273	31.0967	18.0922	15.1742			14.5939	22.9289	169.1360		24.1014	24.0887	22.7939
303	35.3956	21.6375	18.3318			16.8505	25.2318	183.3374		26.3137	26.2194	25.2717
333	39.9795	25.5377	21.7995	19.1279	18.4476	19.1524	27.4776	196.9702	22.2716	28.4970	28.2816	28.3628
363	44.8196	29.7643	25.5525	21.9945	21.5539	21.4916	29.6723	210.1187	24.2580	30.6519	30.2921	31.9994
393	49.8895	34.2823	29.5641	25.1718	24.8681	23.8603	31.8210	222.8547	26.4746	32.7788	32.2631	36.1020
423	55.1655	39.0538	33.8054	28.6440	28.3906	26.2502	33.9281	235.2397	28.8961	34.8783	34.2032	40.5804
453	60.6255	44.0410	38.2467	32.3785	32.1197	28.6534	35.9976	247.3267	31.5004	36.9508	36.1192	45.3336
483	66.2495	49.2081	42.8574	36.3274	36.0522	31.0619	38.0329	259.1620	34.2690	38.9968	38.0158	50.2503
513	72.0192	54.5228	47.6068	40.4319	40.1832	33.4680	40.0372	270.7859	37.1853	41.0166	39.8966	55.2094
543	77.9176	59.9565	52.4649	44.6313	44.5062	35.8647	42.0129	282.2337	40.2353	43.0107	41.7643	60.0800
573	83.9296	65.4845	57.4022	48.8751	49.0137	38.2453	43.9627	293.5368	43.4064	44.9796	43.6208	64.7222
603	90.0408	71.0859	62.3909	53.1368	53.6970	40.6037	45.8886	304.7230	46.6877	46.9236	45.4675	68.9870
633	96.2385	76.7433	67.4046	57.4274	58.5472	42.9344	47.7924	315.8169	50.0694	48.8432	47.3053	72.7168
663	102.5108	82.4422	72.4187	61.8081	63.5553	45.2330	49.6759	326.8408	53.5431	50.7388	49.1349	75.7457
693	108.8468	88.1708	77.4108	66.4028	68.7128	47.4956	51.5406	337.8146	57.1011	52.6106	50.9567	77.8996
723	115.2365	93.9196	82.3605	71.4142	74.0127	49.7190	53.3877	348.7562	60.7366	54.4592	52.7708	78.9967
753	121.6709	99.6809	87.2497	77.1526	79.4497	51.9010	55.2185	359.6819	64.4435	56.2849	54.5773	78.8477
783	128.1416					54.0402	57.0339	370.6064	68.2163	58.0880	56.3761	77.2558
813	134.6408					56.1358	58.8350	381.5431	72.0502	59.8688	58.1669	74.0173
843	141.1617					58.1880	60.6226	392.5041	75.9406	61.6279	59.9496	68.9216
873	147.6976					60.1976	62.3973	403.5007	79.8835	63.3654	61.7237	61.7514
903	154.2428					62.1658	64.1598	414.5428	83.8754	65.0817	63.4890	
933	160.7918					64.0949	65.9107	425.6398	87.9128	66.7772	65.2452	
963	167.3397					65.9874	67.6505	436.8000	91.9927	68.4522	66.9918	
993	173.8819					67.8465	69.3796	448.0312	96.1124	70.1069	68.7285	
1023	180.4143					69.6758	71.0983	459.3402	100.2694	71.7417	70.4551	
1053	186.9331					71.4795	72.8071	470.7334	104.4613	73.3569	72.1711	
1083	193.4348					73.2620	74.5061	482.2162	108.6860	74.9527	73.8763	
1113	199.9163					75.0283	76.1956	493.7938	112.9415	76.5296	75.5704	
1143	206.3747					76.7835	77.8758	505.4706		78.0876	77.2533	
1173	212.8074					78.5333	79.5468	517.2503		79.6272	78.9247	
1203	219.2120					80.2836	81.2088	529.1362		81.1486	80.5845	
1233	225.5864					82.0406	82.8617	541.1311		82.6521	82.2327	
1263	231.9285					83.8111	84.5058	553.2369		84.1378	83.8691	
1293	238.2366					85.6019	86.1409	565.4551		85.6062	85.4939	
1323	244.5091					87.4205	87.7671	577.7868		87.0574	87.1070	
1353	250.7445					89.2747	89.3844	590.2323		88.4916	88.7086	
1383	256.9416					91.1729	90.9928	602.7913		89.9092	90.2989	
1413	263.0993					93.1238	92.5921	615.4629		91.3104	91.8780	
1443	269.2163					95.1371	94.1824	628.2456		92.6953	93.4462	
1473	275.2920					97.2228	95.7634	641.1372		94.0643	95.0039	

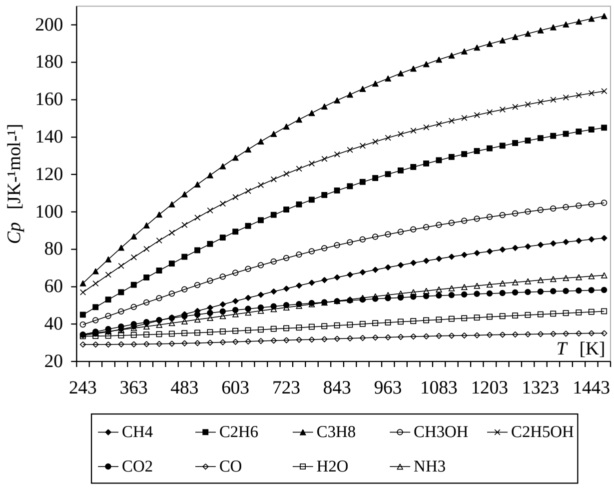

Fig. 5. Isobaric heat capacity (C_p) at different temperatures for important fluids in SOFCs.

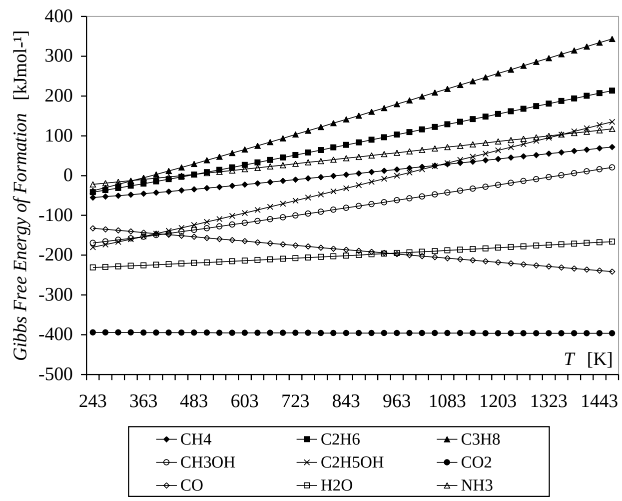

Fig. 8. Gibbs free energy of formation ($\Delta_f G^\circ$) at different temperatures for important fluids in SOFCs.

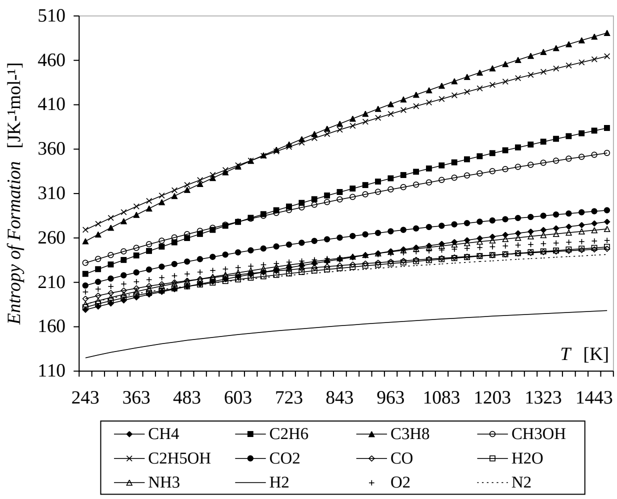

Fig. 6. Entropy of formation ($\Delta_f S^\circ$) at different temperatures for important fluids in SOFCs.

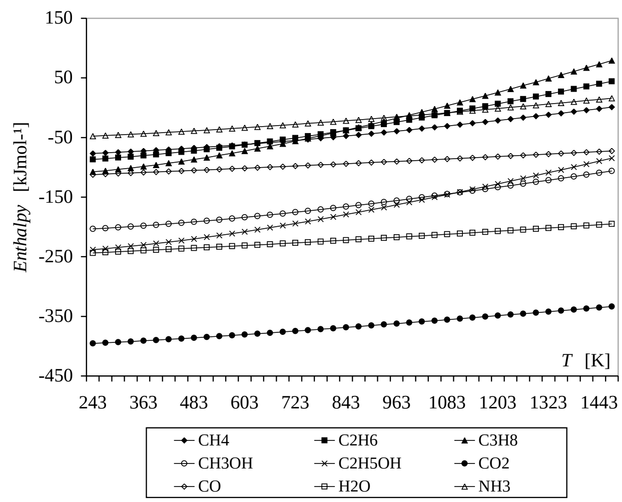

Fig. 9. Enthalpy (H°) at different temperatures for important fluids in SOFCs.

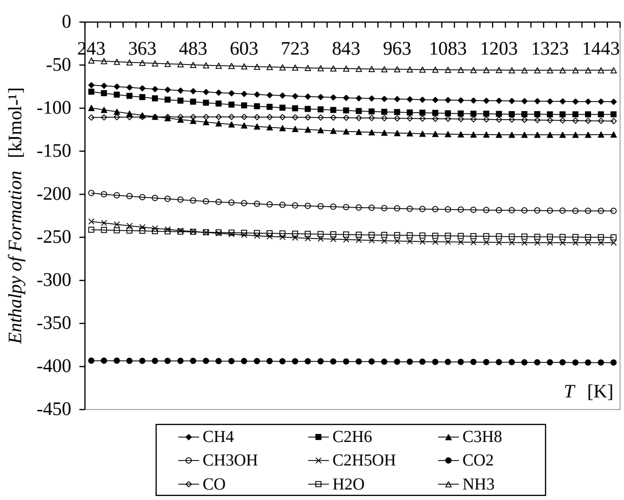

Fig. 7. Enthalpy of formation ($\Delta_f H^\circ$) at different temperatures for important fluids in SOFCs.

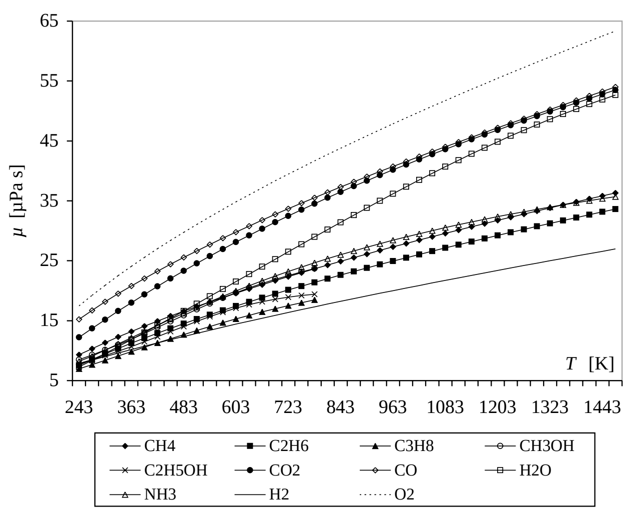

Fig. 10. Viscosity (μ) at different temperatures for important fluids in SOFCs.

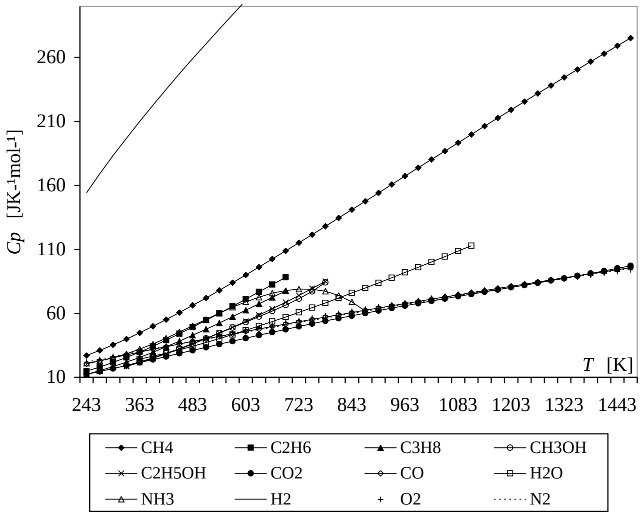

Fig. 11. Thermal conductivity (λ) at different temperatures for important fluids in SOFCs.

5. Thermophysical properties

Finally the isobaric heat capacity (C_p), the entropy of formation (S°),the enthalpy of formation ($\Delta_f H^\circ$), the Gibbs free energy of formation ($\Delta_f G^\circ$), the enthalpy (H°), the viscosity (μ) and the thermal conductivity (λ) are calculated for the fluids reported in Table 1, at different temperatures and 0.1 MPa. The tables are accompanied of their respective figures (Tables 3–9 and Figs. 5–11).

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