

## Evaluation of thermodynamic properties of long-chain organic compounds using GMA equation of state

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Concerning the scientific and industrial importance of long-chain organic compounds, endeavors were made in this research to use a simple and accurate equation of state for prediction of thermodynamic properties of these compounds. Using GMA equation of state, different groups of long-chain organic compounds including alkanes, alcohols, ketones and 1-carboxylic acids were studied. It was concluded and ascertained that GMA equation of state is capable of predicting the density of these compounds with a high degree of accuracy. A more sensitive test for any equation of state is the prediction of differential thermodynamic properties, such as internal pressure, isothermal compressibility and thermal expansion coefficient. In such a test, GMA equation of state predicted these properties with an acceptable degree of accuracy.

**Keywords:** GMA Equation of state; long-chain organic compounds; density; internal pressure; isothermal compressibility

### INTRODUCTION

Long-chain organic compounds are of high importance in different branches of chemistry, including chemical industries. For many scientific and industrial purposes, it is necessary to be able to predict the thermodynamic properties of these compounds. It is not always possible to obtain the required thermodynamic data within the intended range of temperature and pressure from articles which have investigated these compounds experimentally. In such cases an accurate and simple equation of state will be very useful. Goharshadi-Morsali-Abbaspour equation of state (GMA EoS) is a simple and accurate equation which has been used for many compounds including polar, nonpolar fluids, refrigerants, hydrogen-bonded fluids, ionic liquids and mixtures [1-17]. In this research, this equation of state has been used to estimate the density and differential thermodynamic properties of a group of long-chain organic compounds.

Some of the equations of state, although successful in predicting the density, confront with difficulties in predicting differential thermodynamic properties such as internal pressure. The GMA EoS predicts these properties with acceptable accuracy in all cases. In the year 2005, Goharshadi *et al.* [1] derived an accurate and simple equation using the average potential energy. In this work, thermodynamic properties of different groups of long-chain organic compounds, including alkanes, alcohols, ketones

and 1-carboxylic acids were studied using GMA EoS.

### THEORY

The average potential energy is approximately equal to the sum of contributions from nearest neighbors only, assuming single inverse powers for the effective repulsion and attraction.

The GMA equation of state [1] is based on the average potential energy and is given as:

$$(2Z - 1)V_m^3 = A(T) + B(T)\rho \quad (1)$$

where  $Z$ ,  $V_m$ , and  $\rho$  are compressibility factor, molar volume, and molar density, respectively. The intercept and slope of this equation depend on temperature *via* the equations:

$$A(T) = A_0 - 2A_1 / RT + 2A_2 \ln T / R \quad (2)$$

$$B(T) = B_0 - 2B_1 / RT + 2B_2 \ln T / R \quad (3)$$

where  $A_0$ – $A_2$  and  $B_0$ – $B_2$  are constants. To use the equation of state for a liquid, the  $A$  and  $B$  parameters must be known. To find these

parameters, we may plot  $(2Z - 1)V_m^3$  against  $\rho$  for different isotherms. The slope and intercept of the straight lines can be fitted with Eqs. (2) and (3) from which  $A_0$ – $A_2$  and  $B_0$ – $B_2$  can be found, respectively.

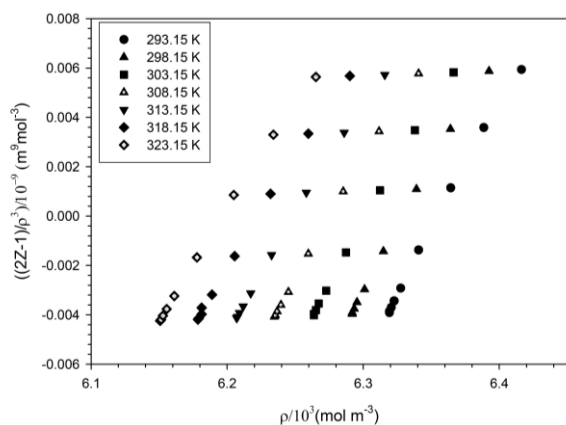
### RESULTS AND DISCUSSION

We used the experimental PVT data for  $C_{18}H_{38}$ ,  $C_{19}H_{40}$  [18],  $C_{20}H_{42}$  [19],  $C_{23}H_{48}$ ,  $C_{24}H_{50}$  [20],  $C_{28}H_{58}$  [21], 1-propanol, 2-propanol, 1-butanol, 2-butanol [22], 1-pentanol, 2-pentanol, 3-pentanol [23], 1-hexanol, 1-octanol, 1-decanol, 1-hexadecanol [24], 1,2-butanediol [25], 2-propanone [26], 2-butanone

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**Table 1.** The average of square of correlation coefficient ( $R^2$ ) of Eq. (1) and the average, minimum, and maximum absolute percent deviations of the calculated densities.

Compound	$T_{\min} - T_{\max}$ (K)	$(P_{\min} - P_{\max})/10^5$ (Pa)	$R^2$	$(100 \times  \rho_{\text{exp}} - \rho_{\text{cal}}  / \rho_{\text{exp}})$ Average (min – max)
C <sub>18</sub> H <sub>38</sub>	313.15-383.15	0.9998-1475.9437	0.9996	0.0533(0.00094-0.28)
C <sub>19</sub> H <sub>40</sub>	313.15-383.15	0.9998-1475.9438	0.9996	0.0532(0.000357-0.27)
C <sub>20</sub> H <sub>42</sub>	373-573	0-4934.2105	0.998	0.631(0.0088-4.36)
C <sub>23</sub> H <sub>48</sub>	333.15-393.15	0.9869-1475.9437	0.9996	0.0502(0.000262-0.0262)
C <sub>24</sub> H <sub>50</sub>	333.15-393.15	0.9869-1475.9438	0.9997	0.0532(0.000357-0.27)
C <sub>28</sub> H <sub>58</sub>	353.15-403.15	0.9869-1475.9439	0.9994	0.062(0.00122-0.3)
1-Propanol	283.15-348.15	0.9869-2048.8527	0.9994	0.07(0.001-0.34)
2-Propanol	283.15-348.15	0.9869-1718.2334	0.9994	0.0761(0.00462-0.431)
1-Butanol	283.15-348.15	0.9869-2034.0489	0.999	0.0478(0.0013-0.23)
2-Butanol	283.15-348.15	0.9869-2037.9965	0.9993	0.079(0.00053-0.45)
1-Pentanol	228.8000-433	98.6923-1973.8465	0.9998	0.038(0.000314-0.166)
2-Pentanol	234-433	98.6923-1973.8465	0.994	0.175(0.00418-1.05)
3-Pentanol	233.6-433	98.6923-1973.8465	0.9994	0.0854(0.0020-0.454)
1-Hexanol	298.15-348.15	0.9869-394.9667	0.9999	0.0089(0.000041-0.003)
1-Octanol	298.15-348.15	0.9869-396.5458	0.9999	0.00635(0.000386-0.018)
1-Decanol	298.15-348.15	0.9869-396.7432	0.9999	0.00538(0.00016-0.019)
1-Hexadecanol	348.15	3.3066-3.4087	0.9999	0.0096(0.0051-0.017)
1,2-Butanediol	288.15-308.15	0.9869-592.154	0.9999	0.00796(0.000737-0.0169)
2-Propanone	278.15-298.15	2.5-389.82	0.9997	0.0540(0.00125-0.472)
2-Butanone	278.15-338.15	25.167-3847.2	0.9911	0.143(0.00166-3.9)
3-Pentanone	278.15-338.15	25.166-3847.2243	0.991	0.147(0.00202-3.9)
2-Hexanone	288.15-338.16	25.1369-3755.835	0.9997	0.107(0.00167-4.2)
1-Butanoic acid	293.15-323.15	0.9869-246.7308	0.9995	0.014(0.000235-0.042)
1-Pentanoic acid	293.15-323.15	0.9869-246.7308	0.9984	0.0258(0.0029-0.061)
1-Hexanoic acid	293.15-323.15	0.9869-246.7308	0.9996	0.033(0.0013-0.075)
1-Heptanoic acid	293.15-323.15	0.9869-246.7308	0.996	0.039(0.0052-0.091)
1-Octanoic acid	293.15-323.15	0.9869-246.7308	0.995	0.042(0.0045-0.091)
1-Decanoic acid	343.15-373.1500	0.9869-88.8231	0.9991	0.00816(0.000102-0.0204)
1-Dodecanoic acid	343.15-373.1500	9.6852-871.6707	0.9997	0.058(0.044-0.073)
1-Tetradecanoic acid	353.15-373.15	0.9869-88.8231	0.9994	0.0063(0.00038-0.018)
1-Hexadecanoic acid	353.15-373.15	0.9869-88.8231	0.9996	0.16(0.14-0.18)



**Fig. 1.** Isotherms of  $(2Z - 1)V_m^3$  versus molar density for 1-octanoic acid

[27], 3-pentanone [28], 2-hexanone [29], 1-butanoic acid, 1-pentanoic acid, 1-hexanoic acid, 1-octanoic acid [30], 1-decanoic acid, 1-dodecanoic acid, 1-tetradecanoic acid and 1-hexadecanoic acid [31] to plot  $(2Z - 1)V_m^3$  against  $\rho$  for each isotherm. Figure 1 shows

isotherms of  $(2Z - 1)V_m^3$  versus  $\rho$  for 1-octanoic acid.

The average values of the square of correlation coefficient ( $R^2$ ) related to 44 compounds are presented in Table 1. As Table 1 shows, the linearity holds very well for all isotherms. Now that the  $A(T)$  and  $B(T)$  parameters are known, the constants  $A0$ – $A2$  and  $B0$ – $B2$  can be obtained using Eqs. (2) and (3). These constants are reported in Table 2.

The first test for every equation of state is its ability in prediction of density. The ability of GMA EOS in the prediction of density and other thermodynamic properties can be evaluated by statistical parameter, namely the absolute average deviation (AAD):

$$AAD = \frac{1}{N} \sum_{i=1}^N 100 \left| \frac{\rho_{\text{exp}} - \rho_{\text{cal}}}{\rho_{\text{exp}}} \right| \quad (4)$$

The average, minimum and maximum AADs of the calculated densities are summarized in Table 1, including the pressure and temperature ranges of the data, the minimum and maximum of  $R^2$ . For most cases, the average AAD is within the range of some

hundredth percent and at the highest limit it is below 0.7%. The AAD values confirm the ability of GMA EOS in density evaluation of long-chain organic compounds from low to high pressures.

A more sensitive test for any equation of state is the prediction of differential thermodynamic properties, such as internal pressure, isothermal

compressibility and thermal expansion coefficient. In this research, the differential thermodynamic properties including internal pressure (Pi), isothermal compressibility ( $\kappa$ ) and thermal expansion coefficient ( $\alpha$ ) were calculated within the ranges where experimental data were available and then were compared with experimental values.

**Table 2.** The constants A<sub>0</sub>–A<sub>2</sub> and B<sub>0</sub>–B<sub>2</sub> obtained using Eqs. (2) and (3).

Fluid	A <sub>0</sub> /10 <sup>-9</sup> (m <sup>9</sup> · mol <sup>-3</sup> )	A <sub>1</sub> /10 <sup>-7</sup> (m <sup>12</sup> · Pa · mol <sup>-4</sup> )	A <sub>2</sub> /10 <sup>-7</sup> (m <sup>12</sup> · Pa · mol <sup>-4</sup> · K <sup>-1</sup> )	B <sub>0</sub> /10 <sup>-9</sup> (m <sup>9</sup> · mol <sup>-3</sup> )	B <sub>1</sub> /10 <sup>-7</sup> (m <sup>12</sup> · Pa · mol <sup>-4</sup> )	B <sub>2</sub> /10 <sup>-7</sup> (m <sup>12</sup> · Pa · mol <sup>-4</sup> · K <sup>-1</sup> )
C <sub>18</sub> H <sub>38</sub>	-264.324	-354.969	1.61E+00	9.16E+01	1.36E+02	-5.53E-01
C <sub>19</sub> H <sub>40</sub>	-256.379	-289.269	1.57E+00	9.43E+01	1.24E+02	-5.71E-01
C <sub>20</sub> H <sub>42</sub>	142.715	707.826	-7.67E-01	-4.54E+01	-2.29E+02	2.48E-01
C <sub>23</sub> H <sub>48</sub>	-1350.43	-2486.71	8.08E+00	5.79E+02	1103.88	-3.45E+00
C <sub>24</sub> H <sub>50</sub>	-1311.42	-2410.37	7.82E+00	6.00E+02	1153.7	-3.56E+00
C <sub>28</sub> H <sub>58</sub>	-1223.19	-1573	7.43E+00	6.47E+02	9.43E+02	-3.88E+00
1-Propanol	0.344705	1.13891	-2.03E-03	-0.0245999	-0.0765579	1.48E-04
2-Propanol	0.681687	1.82242	-4.05E-03	-0.0547893	-0.137487	3.30E-04
1-Butanol	0.488254	2.23432	-2.71E-03	-4.49E-02	-0.187895	2.59E-04
2-Butanol	0.510131	2.21884	-2.87E-03	-3.92E-02	-0.170109	2.28E-04
1-Pentanol	-0.928468	0.215877	5.88E-03	9.69E-02	7.70E-03	-5.93E-04
2-Pentanol	-0.63513	0.906193	4.20E-03	6.75E-02	-6.07E-02	-4.23E-04
3-Pentanol	0.283791	2.86804	-1.26E-03	-2.52E-02	-2.56E-01	1.27E-04
1-Hexanol	1.95191	8.36585	-1.09E-02	-2.26E-01	-0.929727	1.30E-03
1-Octanol	2.04706	16.7522	-9.83E-03	-2.29E-01	-2.19718	1.13E-03
1-Decanol	2.30261	31.9335	-0.0087611	-0.201119	-4.932	6.32E-04
1-Hexadecanol	-0.029164	46.4247	-0.0243929	0.420349	-11.4787	0.00568932
1,2-Butanediol	2.60982	6.79975	-1.56E-02	-0.189351	-0.507765	1.13E-03
2-Propanone	1.96592	3.96434	-1.20E-02	-0.135852	-0.269486	8.31E-04
2-Butanone	1.47699	3.54136	-8.96E-03	-0.134251	-0.301789	8.25E-04
3-Pentanone	1.86212	5.15625	-1.12E-02	-0.184425	-0.483184	1.13E-03
2-Hexanone	1.28495	6.1424	-7.09E-03	-0.153793	-0.672011	8.90E-04
1-Butanoic acid	0.696428	2.59141	-3.95E-03	-0.0548807	-0.204206	3.17E-04
1-Pentanoic acid	0.688818	3.71565	-3.68E-03	-0.0569024	-0.332823	3.12E-04
1-Hexanoic acid	5067.59	11140.8	-3.01E+01	-1544.71	-3387.87	9.19E+00
1-Heptanoic acid	0.907951	8.76561	-4.08E-03	-3.42E-02	-0.928789	8.05E-05
1-Octanoic acid	24.9951	58.2755	-1.50E-01	-3.83894	-8.76538	2.32E-02
1-Decanoic acid	-62.1835	-101.671	3.78E-01	13.1378	22.6667	-7.93E-02
1-Dodecanoic acid	-3085.44	-6074.48	18.5005	729.892	1456.89	-4.37E+00
1-Tetradecanoic acid	2425.26	5321.06	-14.4303	-659.077	-1441.59	3.92E+00
1-Hexadecanoic acid	5067.59	11140.8	-30.1299	-1544.71	-3387.87	9.19E+00

The following equations were used for calculating Pi,  $\kappa$  and  $\alpha$ :

$$P_i = (B_1 + B_2 T) \rho^5 + (A_1 + A_2 T) \rho^4 \quad (5)$$

$$\alpha_P = \frac{(2B_1 + 2B_2 T) \rho^5 + (2A_1 + 2A_2 T) \rho^4 + 2P}{5\rho^5 (RT^2 B_0 - 2B_1 T + 2T^2 B_2 \ln T) + 4\rho^4 (A_0 RT^2 - 2A_1 T + 2A_2 T^2 \ln T) + RT^2 \rho} \quad (6)$$

$$\kappa_T = 2(\rho RT + 4\rho^4 (RTA_0 - 2A_1 + 2TA_2 \ln T) + 5\rho^5 (B_0 RT - 2B_1 + 2B_2 T \ln T))^{-1} \quad (7)$$

**Table 3.** Average, minimum and maximum AAD of calculated isothermal compressibility.

Fluid	$T_{\min} - T_{\max}$ (K)	$(P_{\min} - P_{\max})/10^5$ (Pa)	$(\rho_{\min} - \rho_{\max})/10^3$ (mol · m <sup>-3</sup> )	$(100 \times  \kappa_{\text{exp}} - \kappa_{\text{cal}}  / \kappa_{\text{exp}})$ Average (min – max)
C <sub>18</sub> H <sub>38</sub>	313.15-383.15	0.9998-1475.9437	2.9184-3.2437	2.770809(0.0505358-5.505358)
C <sub>19</sub> H <sub>40</sub>	313.15-383.15	0.9998-1475.9438	2.8104-3.0723	2.671265(0.098203-5.3006)
C <sub>23</sub> H <sub>48</sub>	333.15-393.15	0.9869-1475.9437	2.2559-2.5475	2.596291(0.0223-5.476841)
C <sub>24</sub> H <sub>50</sub>	333.15-393.15	0.9869-1475.9438	2.2090-2.4563	2.353074(0.111-5.426272)
C <sub>28</sub> H <sub>58</sub>	353.15-403.15	0.9869-1475.9439	1.9000-2.1024	2.741533(0.00628-5.27943)
2-Butanone	278.15-338.15	25.167-3847.2	10.5481-12.9608	2.501681(0.0423-5.154782)
3-Pentanone	278.15-338.15	25.166-3847.2243	8.9897-11.0177	1.799331(0.0449-5.912318)
2-Hexanone	288.15-338.16	25.1369-3755.835	7.7323-9.6155	2.973575(0.0731-5.455831)

**Table 4.** Absolute percent deviations of the calculated thermal expansion coefficient

$T(K)$	$\rho/10^3$ (mol · m <sup>-3</sup> )	$\alpha_{\text{exp}} (K^{-1})$	$\alpha_{\text{cal}} (K^{-1})$	$\left  \frac{\alpha_{\text{exp}} - \alpha_{\text{cal}}}{\alpha_{\text{exp}}} \right  \times 100$
C <sub>19</sub> H <sub>40</sub>				
313.15	2.8807	0.000846	0.00085	0.429
323.15	2.8559	0.000864	0.000845	2.162
333.15	2.8309	0.000881	0.00085	3.533
343.15	2.80597	0.000897	0.000862	3.851
353.15	2.7809	0.000912	0.000883	3.190
363.15	2.7556	0.000926	0.000911	1.616
373.15	2.7301	0.00094	0.000948	0.799
383.15	2.7044	0.000954	0.000993	4.053
2-Butanone				
278.15	11.408	0.00124	0.001211	2.306
288.15	11.267	0.00128	0.001265	1.183
298.15	11.1237	0.00131	0.001301	0.652
313.15	10.9062	0.00137	0.001323	3.406
323.15	10.7631	0.0014	0.001316	5.989
338.15	10.56	0.00145	0.001275	12.05
3-Pentanone				
278.15	9.6464	0.00116	0.001136	2.094
288.15	9.5363	0.00118	0.001159	1.814
298.15	9.4257	0.0012	0.001173	2.278
313.15	9.2609	0.00123	0.001177	4.325
323.15	9.1528	0.00124	0.001168	5.783
338.15	8.996	0.00127	0.001139	10.285
2-Hexanone				
278.15	8.2594	0.00105	0.000958	8.735
288.15	8.179	0.00108	0.001	7.410
313.14	7.967	0.00115	0.001102	4.193
C <sub>18</sub> H <sub>38</sub>				
313.15	3.0251	0.000872	0.000866	0.663
323.15	2.998	0.000884	0.000857	3.018
333.15	2.9718	0.000897	0.00086	4.149
343.15	2.9452	0.00091	0.000872	4.166
353.15	2.9184	0.000923	0.000894	3.153
363.15	2.8916	0.000937	0.000926	1.170
373.15	2.8645	0.000951	0.000968	1.775
383.15	2.8372	0.000966	0.00102	5.654

The average, minimum and maximum AAD of calculated isothermal compressibility of some compounds are presented in Table 3. Concerning  $P_i$  and  $\alpha$ , the calculations were done at points where experimental data were available. Calculated  $P_i$  and  $\alpha$  are reported in Tables 4 and 5, respectively.

**Table 5.** Absolute percent deviations of the calculated internal pressure

$T(K)$	$\rho/10^3$ (mol m <sup>-3</sup> )	$P_{i,\text{exp}}/10^5$ (Pa)	$P_{i,\text{cal}}/10^5$ (Pa)	$\left  \frac{P_{i,\text{exp}} - P_{i,\text{cal}}}{P_{i,\text{exp}}} \right  \times 100$
C <sub>19</sub> H <sub>40</sub>				
313.15	2.8807	2957.978	3140.891	6.183
323.15	2.8559	2934.236	3086.592	5.192
343.15	2.80597	2854.51	3028.287	6.087
333.15	2.8309	2897.931	3049.638	5.232
353.15	2.7809	2802.838	3020.877	7.779
363.15	2.7556	2744.981	3025.849	10.232
373.15	2.7301	2681.091	3041.681	13.449
383.15	2.7044	2617.332	3066.978	17.1795
2-Butanone				
278.15	11.408	3392.789	3816.997	12.503
288.15	11.267	3394.618	3850.865	13.440
298.15	11.1237	3345.098	3832.844	14.580
313.15	10.9062	3263.511	3722.332	14.059
323.15	10.7631	3179.169	3603.864	13.358
338.15	10.56	2982.402	3378.232	13.272
3-Pentanone				
278.15	9.6464	3415.695	3571.506	4.561
288.15	9.5363	3210.216	3531.277	10.001
298.15	9.4257	3289.8	3465.893	5.352
313.15	9.2609	3054.782	3327.996	8.943
323.15	9.1528	3052.805	3214.66	5.301
338.15	8.996	2915.976	3021.22	3.609
C <sub>18</sub> H <sub>38</sub>				
313.15	3.0251	2981.571	3126.232	4.851
323.15	2.998	2934.244	3061.715	4.344
333.15	2.9718	2885.551	3019.958	4.657
343.15	2.9452	2830.221	2998.559	5.947
353.15	2.9184	2771.195	2995.318	8.087
363.15	2.8916	2708.795	3008.176	11.051
373.15	2.8645	2643.642	3035.234	14.812
383.15	2.8372	2569.993	3074.648	19.636
2-Hexanone				
278.15	8.2594	3252.268	3088.871	5.0240
288.15	8.179	3201.646	3131.472	2.191
313.14	7.967	3146.949	3173.997	0.859

The average of AAD related to  $\kappa$  is less than 0.03. Concerning  $P_i$  and  $\alpha$ , the average of AAD for all compounds, for which experimental data were available, is less than 0.07. The AAD values in Tables 3, 4 and 5 show that GMA equation of state is able to predict well the differential thermodynamic properties of long-chain organic compound.

## CONCLUSION

The volumetric and other thermodynamic properties of long-chain organic compounds were calculated using GMA EoS over a wide range of temperatures and pressures. The accuracy of GMA EoS in the prediction of density and differential thermodynamic properties was determined using the absolute average deviation (AAD). The results show that GMA EoS can produce the experimental density and differential thermodynamic properties within experimental errors throughout the liquid phase.

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## ОЦЕНКА НА ТЕРМОДИНАМИЧНИТЕ СВОЙСТВА НА ОРГАНИЧНИ СЪЕДИНЕНИЯ С ДЪЛГИ ВЕРИГИ, ПОСРЕДСТВОМ GMA УРАВНЕНИЕ НА СЪСТОЯНИЕТО

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(Резюме)

В това изследване бяха направени усилия, за да се използва просто и точно уравнение на състоянието за предсказване на термодинамичните свойства на органични съединения с дълга верига, отчитайки научното и промишлено значение на тези съединения. Използвайки GMA уравнение на състоянието, различни групи от органични съединения с дълга верига, включително алкани, алкохоли, кетони и 1-карбоксилни киселини бяха изучени. Беше заключено и установено, че GMA уравнението на състоянието е способно да предвижда плътността на тези съединения с висока степен на точност. Един по-чувствителен тест за всяко уравнение на състоянието е прогнозата на диференциални термодинамичните свойства, като вътрешно налягане, изотермичната свиваемост и коефициента на топлинно разширение. В такъв тест, GMA уравнението на състоянието прогнозира тези свойства с приемлива степен на точност.