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MODELING OF THE THERMO-PHYSICAL PROPERTIES OF GRAPES JUICE
I. THERMAL CONDUCTIVITY AND THERMAL DIFFUSIVITY

A.I. Simion[1,2], P. E. Dobrovici[2], L. Rusu[1], L. Gavrila[1]
[1]"Vasile Alecsandri" University of Bacau, Department of Chemical and Food Engineering,
Marasesti no 157, 600115 Bacău, Romania
[2]"Gh. Asachi" Technical University of Iasi, Department of Environmental Engineering and Management, 71 Mangeron Blvd, 700050 Iaşi, Romania
E-mail: asimion@ub.ro

Abstract
The fruit juice processing industry is one of the world's major agro-based businesses. The processing of fruit into juice products requires knowledge of the interplay of many variables. Rationally designed equipment needs a thoroughly knowledge of physical and thermodynamical properties of materials involved: raw materials, additives, intermediate and finished products.
The aim of this work is to establish simple and reliable mathematical relationships between frequent used properties (Π = density, dynamic viscosity, thermal conductivity, thermal capacity, thermal diffusivity) and two key variables: temperature (T) and dry matter content (X) of the grape juice: π = f(T, X).
Using the literature data tables and charts, different regression equations have been tested, in order to get consistent equations that express the studied parameters as a function of temperature and/or dry substance content. The obtained equations are very useful in grapes juice processing technology; they can be used in spreadsheet calculations as in other computer programs.

Keywords: grapes juice, thermo-physical properties, mathematical modeling, food industry

1. INTRODUCTION

Most of the data concerning the properties of materials involved in the fruit juice processing industry are presented in tabular or graphical form [1 – 3]. In these form, experimental data are difficult to use in calculus were properties values are often and repeatedly necessary at different temperatures: fluids' flow, thermal balances, overall heat and/or mass transfer coefficients. Recent research uses artificial neural networking [4] or multiple-parameter models [5] in order to correlate the physical and thermal properties of liquids involved in food processing with their chemical composition. Unfortunately, not all these models meet the two essential requirements for their use in process and process equipment design: (i) reliability and (ii) accuracy for engineering calculations.

2. EXPERIMENTAL PROGRAM

Tabular data (Table 1) and graphic representation (Figure 1 and 2) concerning the variation of grapes juice thermal conductivity and thermal diffusivity variation with dry matter and temperature were used as primary data for the regression analysis. These data were selected due to their wide use in research, development and design of the grapes juice processing industry. The selected data are most often used in fruit juice processing, as required by thermal instability of the product.

Table 1 Variation of grapes juice thermal conductivity with temperatures and dry matter content [2]

Dry matter, [%]	Thermal conductivity $\lambda \cdot 10^2$ [W/(m · K)] at different temperatures T, [K]					
	298	308	318	328	338	348
20	49.1	52.0	53.7	56.5	57.8	59.0
30	45.6	47.3	50.0	52.5	53.8	55.8
40	42.8	45.4	46.8	49.2	50.4	53.2
50	39.8	39.8	41.9	43.9	44.7	49.3
60	37.1	38.2	40.0	41.5	44.0	46.3

Experimental data and different experimental extrapolated equations presented in various scientific papers concerning the variation of thermo-physical properties of grapes juice also were used (Table 2).

Table 2 Equations used in grapes juice thermal conductivity calculus as a function of temperatures (*T*) and dry matter content (*X*) or water content (*w*)

Author	Equation	
Iliescu [2]	water content between 40 and 60%	
	$\lambda = \frac{(1.680 + 0.032) \cdot 10^{-4}}{2.2 - 0.0036 \cdot T} \cdot (1724 - 0.6 \cdot T + 6.3 \cdot w)$	(1)
	water content between 60 and 96%	
	$\lambda = \frac{(0.320 + 0.055) \cdot 10^{-4}}{2.2 - 0.0036 \cdot T} \cdot (1585 - 0.6 \cdot T + 4 \cdot w)$	(2)
Moyseev [6]	$\lambda = \left[0.154 + 0.16 \cdot \left(\frac{X}{100}\right) - 0.32 \cdot \left(\frac{X}{100}\right)^2\right] \cdot \frac{1.16 \cdot (T - 273)}{100} + 0.254 \cdot \left(\frac{X}{100}\right)^{-0.225} \cdot 1.16$	(3)
Riedel [7]	$\lambda = [0.565 + 0.0018 \cdot (T - 273) - 0.000006 \cdot (T - 273)^2] \cdot (1 - 0.0054 \cdot X)$	(4)

Frequently thermo-physical properties of various products in the food industry are not presented as numerical data but in graphics forms. Therefore xyExtract Graph Digitizer.v2.3 software was used to extract numerical data from graphical representations.

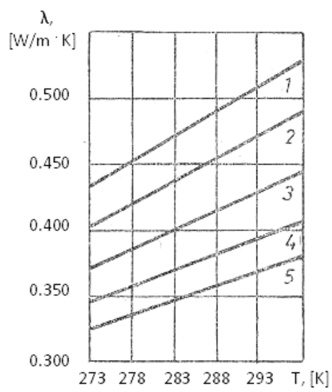

Figure 1. Thermal conductivity variation with temperature at different dry matter (X) content: 1 – 20%, 2 – 30%, 3 – 40%, 4 – 50%, 5 – 60%

The data were plotted in *Temperature – Thermo-physical property, Dry matter content – Thermo-physical property* coordinates and linear regression techniques, involving least square method were used to reveal the best-fit equation. Microsoft Excel™ 2007 spreadsheets and CurveExpert® software were used for equations' establishing.

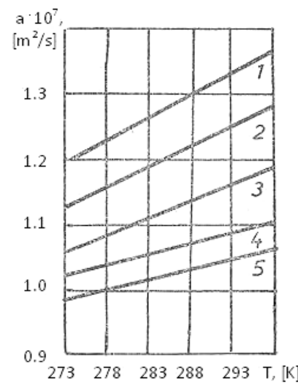

Figure 2. Thermal diffusivity variation with temperature at different dry matter (X) content: 1 – 20%, 2 – 30%, 3 – 40%, 4 – 50%, 5 – 60%

3. RESULTS AND DISCUSSIONS

3.1 Thermal conductivity

Using Microsoft Excel™ 2007 spreadsheets and CurveExpert® software, a logarithmic correlation between temperature and thermal conductivity, at constant dry matter content has been established:

$$\lambda = -A + B \ln T \quad (5)$$

The *A* and *B* values are presented in Table 3. The regression coefficients R^2 are greater than 0.97, thus indicating a good correlation of variables.

Table 3. Coefficients for equation 5

Dry matter, [%]	*A*	*B*	R^2
20	-3.17179	0.643777	0.9829
30	-3.11794	0.627733	0.9893
40	-2.98474	0.599536	0.9935
50	-3.01122	0.598408	0.9914
60	-3.03071	0.595982	0.9773

In order to correlate *A* and *B* coefficients with dry matter content, more models were used in CurveExpert® software (1st, 2nd and 3rd degree polynomial equations, "vapor pressure" model, "heat capacity" model etc.). The best fit model is the 2nd degree polynomial equation with good regression coefficients (Table 4).

$$Coefficient = a \cdot X^2 + b \cdot X + c \qquad (6)$$

Table 4. Coefficients for equation 6

Coeff.	*a*	*b*	*c*	R^2
A	-0.00022	0.021394	-3.52518	0.8835
B	0.000039	-0.00435	0.717358	0.9583

Combining the equations 5 and 6 and replacing the coefficients with numeric values, the final form of proposed equation model is:

$$\lambda = -(-0.00022 \cdot X^2 + 0.021394 \cdot X - 3.52518) + (0.000039 \cdot X^2 - 0.00435 \cdot X + 0.717358) \cdot \ln T \qquad (7)$$

The obtained empiric equation correlates thermal conductivity of grape juice with temperature in range of 273 and 348 K and dry matter content between 20 and 60%.
Using the equations (1), (2), (3), (4) and (7) in grape juice thermal conductivity calculus, the results were compared with published experimental values (Table 1).
To quantify the deviation from experimental data, between measured and calculated thermal conductivities, the relative error was used:

$$\varepsilon = \left(\frac{\lambda_{measured} - \lambda_{calculated}}{\lambda_{measured}} \right) \cdot 100 \quad [\%] \qquad (8)$$

By analyzing the values of induced relative error for each used formula it can be observed that for the proposed equation model the relative average error is only -0.05% comparatively with 3.145% at Moyseev's equation and -4.975% at Riedel's equation (Table 5).
The calculated values graphic representations were presented in Figures 3 – 7. Because of induced relative error over 50% for some values, the Iliescu's equations were removed from graphical representation.

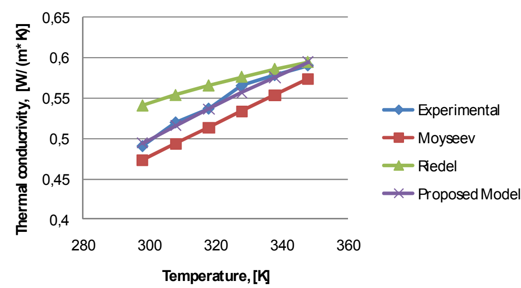

Figure 3. Thermal conductivity of grapes juice with 20% dry matter content

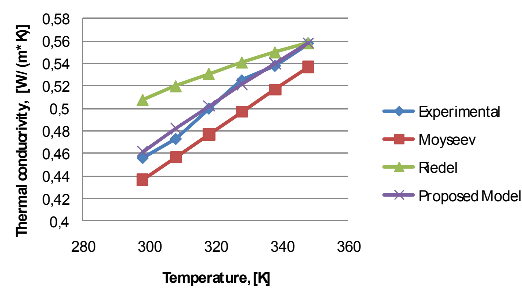

Figure 4. Thermal conductivity of grapes juice with 30% dry matter content

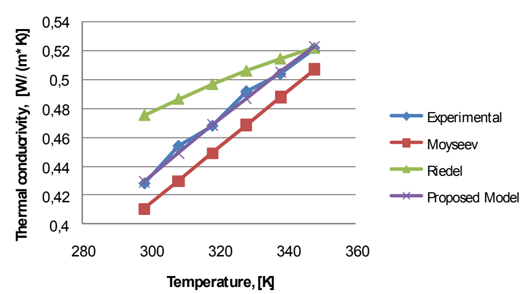

Figure 5. Thermal conductivity of grapes juice with 40% dry matter content

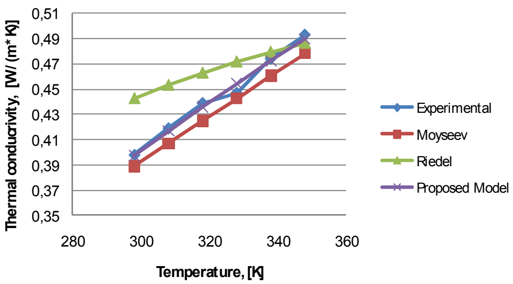

Figure 6. Thermal conductivity of grapes juice with 50% dry matter content

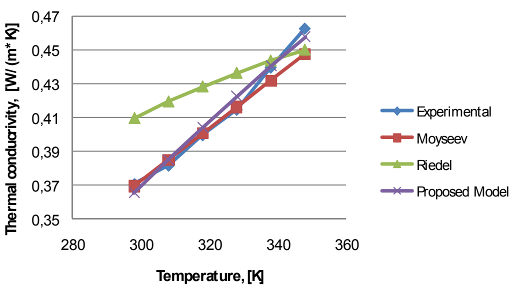

Figure 7. Thermal conductivity of grapes juice with 60% dry matter content

3.2 Thermal diffusivity

Because literature [1-3] recommends a single formula for calculating the grape juice thermal diffusivity, only applicable for dry matter content between 60 and 90%, the graphic representation was used for extract numerical data with xyExtract Graph Digitizer.v2.3 software to offer an empirical model.

Table 5. Comparison between measured and calculated thermal conductivity of grapes juice

Temperature, [K]	Dry matter, [%]	Thermal conductivity, λ [W/(m·K)]								
		Experimental [2]	calculated with equation:							
			1 and 2		3		4		7	
			λ	ε [%]	λ	ε [%]	λ	ε [%]	λ	ε [%]
298	20	0.491	-	-	0.473442	3.576	0.540775	-10.137	0.494555	-0.724
	30	0.456	-	-	0.436541	4.267	0.508038	-11.412	0.461651	-1.239
	40	0.428	0.292097	31.753	0.410472	4.095	0.4753	-11.051	0.429184	-0.277
	50	0.398	0.282529	29.013	0.389029	2.254	0.442563	-11.197	0.397155	0.212
	60	0.371	0.041459	88.825	0.36962	0.372	0.409825	-10.465	0.365562	1.466
308	20	0.52	-	-	0.493533	5.090	0.55362	-6.465	0.515875	0.793
	30	0.473	-	-	0.456632	3.460	0.520105	-9.959	0.482178	-1.940
	40	0.454	0.300792	33.746	0.429821	5.326	0.48659	-7.178	0.449175	1.063
	50	0.419	0.290908	30.571	0.406893	2.890	0.453075	-8.132	0.416868	0.509
	60	0.382	0.042621	88.843	0.385256	-0.852	0.419559	-9.832	0.385255	-0.852
318	20	0.537	-	-	0.513624	4.353	0.565394	-5.288	0.536513	0.091
	30	0.5	-	-	0.476723	4.655	0.531166	-6.233	0.502048	-0.410
	40	0.468	0.310081	33.743	0.449169	4.024	0.496938	-6.183	0.468528	-0.113
	50	0.439	0.29986	31.695	0.424757	3.245	0.462711	-5.401	0.435951	0.694
	60	0.4	0.043861	89.035	0.400893	-0.223	0.428483	-7.121	0.404319	-1.080
328	20	0.565	-	-	0.533716	5.537	0.576098	-1.964	0.556512	1.502
	30	0.525	-	-	0.496815	5.369	0.541222	-3.090	0.521304	0.704
	40	0.492	0.320026	34.954	0.468518	4.773	0.506346	-2.916	0.487281	0.959

	50	0.447	0.309443	30.773	0.442621	0.980	0.471471	-5.474	0.454444	-1.665
	60	0.415	0.04519	89.111	0.41653	-0.369	0.436595	-5.204	0.422792	-1.878
338	20	0.578	-	-	0.553807	4.186	0.585732	-1.338	0.57591	0.362
	30	0.538	-	-	0.516906	3.921	0.550273	-2.281	0.539981	-0.368
	40	0.504	0.330699	34.385	0.487867	3.201	0.514814	-2.146	0.505471	-0.292
	50	0.474	0.319729	32.547	0.460485	2.851	0.479355	-1.130	0.472381	0.342
	60	0.44	0.046616	89.406	0.432167	1.780	0.443895	-0.885	0.44071	-0.161
348	20	0.59	-	-	0.573898	2.729	0.594295	-0.728	0.594743	-0.804
	30	0.558	-	-	0.536997	3.764	0.558318	-0.057	0.558113	-0.020
	40	0.522	0.342183	34.448	0.507216	2.832	0.52234	-0.065	0.52313	-0.217
	50	0.493	0.330796	32.901	0.478349	2.972	0.486363	1.346	0.489795	0.650
	60	0.463	0.04815	89.600	0.447804	3.282	0.450385	2.725	0.458106	1.057

Using Microsoft Excel™ 2007 software, a linear correlation between temperature and thermal diffusivity at constant dry matter content has been established:

$$a = M + N \cdot T \qquad (9)$$

The *M* and *N* values are presented in Table 6.

Table 6. Coefficients for equation 9

Dry matter. [%]	*A*	*B*	R^2
20	-0.66939	0.006829	0.998
30	-0.531971	0.006086	0.999
40	-0.401552	0.005343	0.995
50	0.0968	0.0034	0.994
60	0.161878	0.003034	0.972

In order to correlate *M* and *N* coefficients with dry matter content more models were used in CurveExpert® software (1st, 2nd and 3rd degree polynomial equations, “vapor pressure” model, “heat capacity” model etc.). The best fit model is the 2nd degree polynomial equation with good regression coefficients (Table 7).

$$Coefficient = s \cdot X^2 + v \cdot X + u \qquad (10)$$

Table 7. Coefficients for equation 10

Coeff.	*s*	*v*	*u*	R^2
A	0.0001595	0.01015587	-0.962119	0.933
B	-3.2E-07	-7.727E-05	0.0086028	0.957

Combining the equations 9 and 10 and replacing the coefficients with numeric values, the final form of proposed equation model is:

$$a = -(0.0001595 \cdot X^2 + 0.01015587 \cdot X - \\ - 0.962119) + (-3.2E-07 \cdot X^2 - \\ - 7.7274E-05 \cdot X + 0.0086028) \cdot T \qquad (11)$$

The obtained empiric equation correlates thermal diffusivity of grape juice with temperature in range of 273 and 298 K and dry matter content between 20 and 60%.

By analyzing the values the induced relative error for proposed equation model is only -0.11% in average (Table 8).

A graphic representation of proposed model is not required because the values used for conceiving this model were extracted from another literature offered graphic.

Table 8. Comparison between measured and calculated thermal diffusivity of grapes juice

Temperature, [K]	Dry matter, [%]	Thermal diffusivity, *a* [m²/s]		
		Experimental [2]	calculated with equation 11:	
			a	*ε* [%]
273	20	1.195	1.19664	-0.13726
	30	1.13	1.123484	0.576667
	40	1.06	1.064825	-0.45515
	50	1.025	1.020663	0.423131
	60	0.983	0.990999	-0.8137

278	20	1.23	1.23129	-0.10484
	30	1.16	1.153473	0.562688
	40	1.08	1.089835	-0.91064
	50	1.04	1.040376	-0.03614
	60	1.012	1.005096	0.682253
283	20	1.26	1.265939	-0.47134
	30	1.19	1.183462	0.549414
	40	1.11	1.114845	-0.43651
	50	1.06	1.060089	-0.00837
	60	1.023	1.019193	0.372189
288	20	1.3	1.300588	-0.04525
	30	1.22	1.213451	0.536793
	40	1.14	1.139856	0.012668
	50	1.08	1.079802	0.018363
	60	1.037	1.033289	0.357819
293	20	1.33	1.335238	-0.39381
	30	1.25	1.24344	0.524777
	40	1.16	1.164866	-0.41948
	50	1.09	1.099515	-0.8729
	60	1.051	1.047386	0.343832
298	20	1.366	1.369887	-0.28456
	30	1.283	1.273429	0.745952
	40	1.193	1.189876	0.261839
	50	1.11	1.119228	-0.83131
	60	1.063	1.061483	0.142687

4. CONCLUSIONS

Since computer based programs or spreadsheets require correlation equations of the thermal properties of materials with state parameters (temperature and concentration) some regression equations that correlate grapes juice thermal conductivity and diffusivity with temperature and dry matter content were established.

The proposed equation in thermal conductivity is valid for temperatures between 273 – 348 K and dry matter content of 20 – 60%. For thermal diffusivity the proposed equation is valid in 273 – 298 K temperature range and dry matter content of 20 – 60%.

5. REFERENCES

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