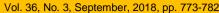
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# Application GMDH artificial neural network for modeling of Al<sub>2</sub>O<sub>3</sub>/water and Al<sub>2</sub>O<sub>3</sub>/Ethylene glycol thermal conductivity

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#### **ABSTRACT**

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### Keywords:

nanofluid, thermal conductivity, GMDH, artificial

Thermal conductivity of nanofluids depends on several parameters including temperature, concentration, and size of nanoparticles. Most of the proposed models utilized concentration and temperature as influential factors in their modeling. In this study, group method of data handling (GMDH) artificial neural networks is applied in order to model the dependency of thermal conductivity on the mentioned factors. Firstly, temperature and concentration considered as inputs and a model is represented. Afterwards, the size of nanoparticles is added to the input variables and the results are compared. Based on obtained results, GMDH is an appropriate method to predict thermal conductivity of the nanofluids. In addition, it is necessary to consider size of nanoparticles in order to have a more precise model.

#### 1. INTRODUCTION

Nanotechnology utilization developed in recent years due to their ability to enhance efficiency of energy systems and decrease the size of tools. By applying nanotechnology it is possible to obtain materials with more favorable properties such as mechanical strength, electrical conductivity, thermal conductivity and etc. [1–3]. By applying nanotechnology, the nanofluids are obtained which can be very appropriate for various purposes, especially in heat transfer and thermal processes [4–9].

Nanofluids are prepared by dispersion of particles with nano scale dimension in a base fluid [10–13]. Nanofluids are widely used in heat transfer applications due to their higher thermal conductivity compared with the base fluids [14-15]. Improvement in thermal conductivity of nanofluids is attributed to high surface/volume ratio of nano particles [10, 16]. Several studies have focused on utilization of nanofluids for heat transfer applications [17–20]. Using nannofluids can significantly enhances heat transfer in comparison with pure fluids. Improvement in thermal performances is mainly attributed to higher thermal conductivity of nanofluids in comparison with the base fluid [21].

Rashidi et al. [22] used CuO,  $Al_2O_3$ ,  $TiO_2$  nano particles in turbine oil to investigate the effect of adding the mentioned nano particles on heat transfer. Results revealed that using the nano particles led to enhancement in heat transfer coefficient. Tabari et al. [23] conducted a study on application of multiwalled carbon nano tubes (MWCNTs)/water in a heat exchanger. Obtained results indicated that using the nanofluid

enhance convective heat transfer compared with using the base fluid. In addition to convective heat transfer, applying nanofluids can enhance boiling heat transfer [24-25]. Minakov et al. [26] applied various nano particles including silicon, aluminum, iron oxide and diamond in distilled water and compared boiling heat transfer on cylindrical heater. Results showed that using nanofluids can enhance critical heat flux which was mainly attributed to deposition of nano particles on the surface of the heater. Dadjoo et al. [27] compared pool boiling of  $SiO_2$ / water and water on a flat plate heater. Obtained data revealed that the boiling heat transfer coefficient improved by using nanofluid; however, there was an optimal concentration for improvement in heat transfer.

Nano particles dispersion in a base fluid change its thermophysical specifications [28–33]. Changes in thermophysical properties of nanofluids depend on several factors including size and shape of nano particles, their concentration, and temperature of the nanofluid [34–40]. Among various thermphysical properties, thermal conductivity and dynamic viscosity play more important role in thermal behavior of the nanofluids [41]. Several studies have concentrated on the effect of adding nano particles on dynamic viscosity and thermal conductivity of nanofluids [42-46].

Since the cost of experimental research is high in some cases, predicting the thermal conductivity of the nanofluid before testing will reduce the cost and time and provide a detailed experimental design. Hence, in recent years, the prediction of thermal properties of nanofluid with different mathematical methods has been carried out. Nadooshan et al

[47] experimentally measured viscosity of  $SiO_2 - MWCNTs$ / 10W40 engine oil and applied artificial neural network in order to predict the viscosity. In the proposed model, shear rate, temperature and concentration solid phase were considered as input variable for the model. Experimental results indicated that the r elative viscosity increased by increasing the concentration of solid phase. The proposed model had good agreement with experimental data and its Rsquared value was 0.9948. Alirezaie [48] et al experimentally investigated the effects of concentration, temperature and shear rate on the dynamic viscosity of MWCNT (COOH-Functionalized)/MgO- engine oil. Results showed that dynamic viscosity increased by solid volume concentration increment and decreased by temperature increase. In addition, a correlation was proposed and compared with artificial neural network model to predict the viscosity. Based on the results, artificial neural network showed higher accuracy in modeling. In another study, three artificial neural network approaches including Genetic Algorithm-Radial Basis Function Neural Networks (GA-RBF), Least Square Support Vector Machine (LS-SVM) and Gene Expression Programming (GEP) were utilized to predict dynamic viscosity of TiO2 / SAE 50 nanofluid [49]. The results of the models indicated that GA-RBF method had the best accuracy among the applied approaches.

In addition to models proposed for predicting dynamic viscosity of nanofluids, there are some studies which have focused on thermal conductivity of nanofluids [50]. Hemmeat Esfe et al. [51] experimentally assessed ZnO-MWCNT/EGwater thermal conductivity and utilized artificial neural network to model the thermal conductivity. The effects of temperature and concentration were considered in this study. The volume fraction of solid was in the range of 0.02 to 1% and the temperature varied between 30 and 50 °C Results indicated that the thermal conductivity ratio of nanofluids increased by increasing the temperature and volume fraction of solid phase. Afrand et al. [52] proposed a correlation by using curve fitting and design an artificial neural network to predict thermal conductivity of MgO/water nanofluids. The input variables were temperature and nano particles concentration in the base fluid. Comparison between the outputs of neural network model and the proposed correlation revealed that the accuracy of the artificial neural network model was higher than the empirical correlation.

Based on literature review, artificial neural network modeling is an appropriate tool to model and predict thermal conductivity of nanofluids. Most of the conducted studies have considered temperature and concentration as influential parameters and input variables [53–57]; however, the size of nano particles affect thermal conductivity of nanofluids. In this study, group method of data handling (GMDH) artificial neural network is applied in order to model thermal conductivity ratio of  $Al_2O_3$  /water and  $Al_2O_3$ /EG because  $Al_2O_3$  nanofluid is a usual nanofluid. The applied algorithm in this study is novel and powerful for modeling to determine the relationship of  $Al_2O_3$  nanoparticles concentration, size and fluid temperature to nanofluid thermal conductivity of water and ethylene glycol as a coolant fluid.

### 2. METHOD

GMDH artificial neural network is an accurate and powerful predictive approach which is applicable for modeling of

engineering systems and recognition of patterns. GMDH is a self-orgnizing network and one-directional. There are various layers in these types of networks and the neurons contain 1 output and 2 inputs as illustrated in figure 1. The neurons have one bias and 5 weights.



Figure 1. Structure of neuron in GMDH

In order to correlate inputs and output in each layer, Volterra functional series are used. Details about this algorithm and working principles are presented in ref [56].

### 3. RESULTS AND DISCUSSION

T In order to model the thermal conductivity ratio of the nanofluids, GMDH method is applied. In the first step, the thermal conductivity ratio of the nanofluids is considered as a function of temperature and volumetric concentrations. Afterwards, the size of nano particles added to the input variables and the results are compared with each other. Ranges of each parameter are represented in tables 1 & 2.

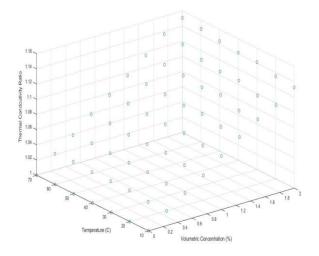
**Table 1.** Ranges of parameters for  $Al_2O_3$ /water nanofluid

Parameter	Range
Temperature (°C)	10-70
Volumetric concentration (%)	0-4
Average size of nano particles (nm)	5-282

**Table 2.** Ranges of parameters for  $Al_2O_3$ /EG nanofluid

Parameter	Range
Temperature (°C)	10-70
Volumetric concentration (%)	0.25-5
Average size of nanoparticles (nm)	2-53

## 3.1. Applying GMDH method by using temperature and concentration



**Figure 1.** Thermal conductivity ratio vs temperature and concentration for  $Al_2O_3$ /water nanofluid [61]

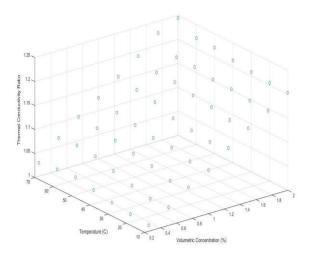


Figure 2. Thermal conductivity ratio vs temperature and concentration for  $Al_2O_3$ /EG nanofluid [61]

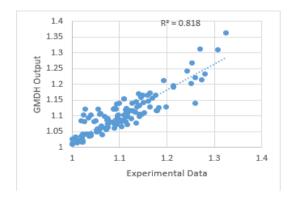
Based on the literature review, thermal conductivity of nanofluids increase as the temperature or/and concentration increase. Various studied investigated the effect of temperature on thermal conductivity of nanofluids [58-59]. Improvement in thermal conductivity by temperature increase is attributed to the Brownian motion and nano structures' thermophoresis behavior [60]. Moreover, increase in concentration of nano particles increases thermal conductivity due to higher thermal conductivity of solid particles in comparison with the base fluids. Figures 2 & 3 show the results of a study conducted by Agarwal et al. [61] which investigated the effects of temperature and concentration on the thermal conductivity of alumina nano particles in water and EG.

In order to utilize GMDH method for predicting thermal conductivity ratio of the nanofluids, data are extracted from experimental data represented in Refs [61–70]. By applying the GMDH method, thermal conductivity ratio obtained as below:

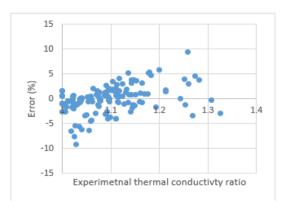
### Thermal Conductivity Ratio = -0.0115572 + N17\*0.645631 + N71\*0.364922

The calculation procedure of coefficient is represented in appendix 1.

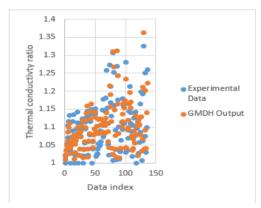
The obtained results by considering temperature and concentration as input variables in GMDH method, are shown in figures 4 to 6 for the water-based nanofluid.



**Figure 3.** Experimental data vs GMDH output for thermal conductivity ratio of  $Al_2O_3$ /water nanofluid



**Figure 4.** Error for various values of thermal conductivity ratio of  $Al_2O_3$ /water nanofluid



**Figure 5.** Comparison between experimental data and GMDH output for  $Al_2O_3$ /water nanofluid

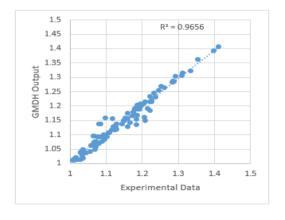
The R-squared and RMSE values for the proposed model by considering temperature and concentration as input variables are 0.818 and 0.0306, respectively. These values show that the proposed model is not appropriate for prediction and the input variables are not adequate.

In addition to water – based nanofluid, thermal conductivity ratio of the  $Al_2O_3$ /EG nanofluid is obtained by considering temperature and concentration as input variables.

Obtained results by applying GMDH method are compared with experimental data in figures 7 to 9.

### Thermal conductivity ratio = $-0.119797 - N196^2*0.0907248 + N6*1.20918$

The calculation procedure of coefficient is represented in appendix 2.



**Figure 6.** Experimental data vs GMDH output for thermal conductivity ratio of  $Al_2O_3$ /EG nanofluid

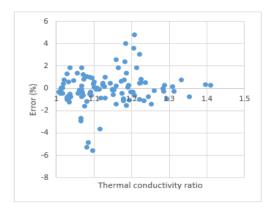


Figure 7. Error for various values of thermal conductivity ratio of  $Al_2O_3$ /EG nanofluid



**Figure 8.** Comparison between experimental data and GMDH output for  $Al_2O_3$ /EG nanofluid

The R-squared and RMSE values for the proposed model for  $Al_2O_3$ /EG nanofluid are 0.965 and 0.017, respectively.

### 3.2. Applying GMDH method by using temperature, concentration and size of nanoparticles

In addition to temperature and concentration, the size of nanoparticles is another influential parameter on thermal conductivity. The majority of studies concluded that the increase in particle size leads to enhancement in thermal conductivity; however, there must be an optimal size for nanoparticles and the improvement in thermal conductivity is not unlimited [71].

By considering size, temperature and concentration of nanofluid, the results are obtained more accurately as shown in figures 10 to 12. The obtained regression fit obtained as:

## Thermal conductivity ratio = -0.033918 + N189\*N2\*4.82245 - N189^2\*2.41237 + N2\*1.05937 - N2^2\*2.4346

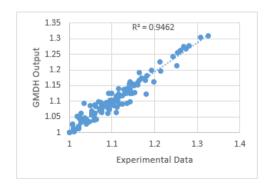
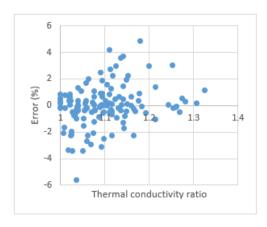
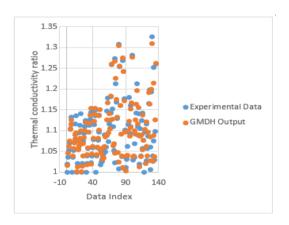


Figure 9. Experimental data vs GMDH output for thermal conductivity ratio of  $Al_2O_3$ /water nanofluid



**Figure 10.** Error for various values of thermal conductivity ratio of  $Al_2O_3$ /water nanofluid



**Figure 11.** Comparison between experimental data and GMDH output for  $Al_2O_3$ /water nanofluid

The calculation procedure of coefficient is represented in appendix 3.

By comparing the results of GMDH output with and without considering particle size, it is concluded that using particle size as one of the input variables leads to obtain more accurate regression. The R-squared and RMSE in this condition are equal to 0.9462 and 0.0166. The maximum error for predicted data by applying GMDH method and considering temperature, size and concentration as input variables is less than 6% which shows the accuracy of the proposed model.

The proposed model by using GMDH approach for  $Al_2O_3$ /EG nanofluid by considering three input variables (size, temperature and concentration) obtained as:

### Thermal conductivity ratio = -0.000286792 + N12\*0.560308 + N23\*0.439945

The calculation procedure of coefficient is represented in appendix 3.

Comparison between obtained results by GMDH method and experimental data are and RMSE values are equal to 0.9958 and 0.0059, respectively.

### 4. CONCLUSION

In this study, GMDH artificial neural network was applied in order to propose a model for thermal conductivity ratio of  $Al_2O_3$ /water and  $Al_2O_3$ /EG nanofluids. Firstly, temperature and concentration were considered as input variables for the

model. Obtained R-square values based on 2-variable model, were 0.818 and 0.965 for  $Al_2O_3$ /water and  $Al_2O_3$ /EG, respectively. Since the size of nanoparticles is an influential parameter on thermal conductivity ratio of nanofluids, particle size added to input variables in the second stage to compare results. Based on obtained results, the R-square values of the proposed models by considering three variables (size, temperature and concentration), were 0.9462 and 0.9958, respectively. Results indicated that the models with three input variables were more precise and applicable.

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### **APPENDIX 1**

```
N71 = 1.06079 - N259*2.58978 + N259*N209*0.792102 +
N209*1.75108
N209 = 5.02276 - N261*3.50572 + N261*N299*4.10165 -
N299*4.583
N299
             1.03691
                            concentration*0.924928
concentration*N304*0.871805
            1.04253
                            temperature*0.0320422
temperature*N302*0.030704
N259 = 3.48693e-12 + N269*1
N17 = -2.4818 - N266*N167*2.05063 + N167*5.51865
N167 = 0.407857 + N250*0.211268 + N250*N292*0.379164
N292 = 32.9059 - N302*30.4682 + N302*N304*28.6923 -
N304*30.0018
N304 = 1.47349 + temperature*0.0418532 - temperature*
\sqrt[3]{\text{temperature}} *0.00705606 - \sqrt[3]{\text{temperature}} *0.313222
N250 = 0.0320969 + N269*2.65972 - N279*1.68903
           1.06924 - temperature*0.00119483
N269 =
temperature*concentration*0.00169259
concentration*0.0211386
N266 = -2.29609 + N279*2.91761 - N279*N302*1.82553 +
N302*2.18258
N302 = 0.997978 + concentration*0.107522 - concentration*
<sup>3</sup>√concentration
                   *0.0429876
                                + <sup>3</sup>√concentration
*0.00726233
N279 = 1.14644 - concentration*0.130648 + concentration*
```

### Appendix 2

```
N6 = 0.131852 + N42^2*0.0983067 + N23*0.77152

N23 = -0.493869 + N241*N36*47.0535 - N241^2*23.7864 + N36*1.83383 - N36^2*23.6136

N36 = -0.00345911 + N68*0.450018 + N105*0.553037

N105 = -0.130651 + N235*1.96563 + N235*N129*110.748 - N235^2*56.3859 - N129*0.759341 - N129^2*54.438

N129 = -0.167899 - N192*0.788695 - N192*N221*110.346 + N192^2*55.8412 + N221*2.11734 + N221^2*54.3414

N235 = 0.164618 - N300*2.33927 - N300*N323*2.28051 + N300^2*2.40457 + N323*3.05147

N300 = 1.21581 - concentration^2*0.00173893 - N319*1.20054 + N319^2*0.994582

N68 = 0.587159 - N142*N151*70.1059 + N142^2*35.1058 + N168^2
```

 $\sqrt[3]{\text{temperature}} *0.0518859 - \sqrt[3]{\text{temperature}} *0.0363114$ 

```
N151^2*35.4198
N151 = -0.00441004 + N192*0.46583 + N217*0.538064
N192 = 0.394507 + N241*0.312121 + N241*N292*0.29795
N142 = 0.470252 + N220*14.4813 - N220*N221*249.946 +
N220^2*119.131 - N221*14.2949 + N221^2*131.16
N221 = 0.180833 + N252*13.4003 - N252*N285*194.021 +
N252^2*91.5259 - N285*12.6991 + N285^2*102.613
N220 = 0.425837 - concentration*N252*0.0185734 +
N252^2*0.574913
N252 = 0.347598 - N321*3.31529 - N321*N324*2.89701 +
N321^2*3.1634 + N324*3.70363
N241 = 1.35933 - \sqrt[3]{temperature}
                                        *0.534273
<sup>3</sup>√temperature
                 *N324*0.32958
                                       3 temperature
^2*0.0307514 - N324^2*0.0287977
N42 = 0.00779353 - N303*0.285346 + N71*1.27846
N71 = 0.0793258 - N156*N186*70.8774 + N156^2*35.7131
+ N186*0.86692 + N186^2*35.2173
N186 = 0.0296152 - N198*N231*128.519 + N198^2*64.6399
+ N231*0.969541 + N231^2*63.8781
N231 = 0.580762 - N256*N293*172.682 + N256^2*86.8381
+ N293^2*86.2675
N293 = 0.23575 + N317*0.589705 + N319^2*0.17737
N198 = 0.411202 + N236*0.283245 + N236*N292*0.310356
N292 = 1.98271 + \sqrt[3]{concentration} *0.704065
\sqrt[3]{concentration} *N318*0.574967 - N318*3.01295 +
N318^2*1.95251
N236 =
            0.433692 - temperature*0.0128194
temperature*N324*0.0112107 + temperature^2*1.65897e-05
+ N324*0.597218
N156 = -0.00515273 + N210*0.415879 + N217*0.58867
N217 = -0.585315 + N285*35.1752 + N285*N298*1092.37
N285^2*561.779 - N298*33.2139 - N298^2*530.969
N285 = 0.577866 + N318*N319*0.429767
N319 = 1.02129 - temperature*0.00394802 + temperature*
\sqrt[3]{concentration} * 0.00316982 + temperature^2*2.19221e
05 + \sqrt[3]{concentration} ^2*0.0750819
N318 = 1.4061 + concentration*<sup>3</sup> temperature* 0.032136
concentration^2*0.00798288 - \sqrt[3]{temperature} *0.250409 +
"temperature, cubert"^2*0.0376592
N210 = 0.577324 + N245*N256*0.430174
N256 = 0.158917 - N317*1.03499 - N317*N324*1.19101 +
N317^2*1.31551 + N324*1.75224
N245 = 91.6158 - N324*15.1293 + N324*N327*14.258 -
N327*147.5 + N327^2*58.7891
N303 = 0.00176952 - \sqrt[3]{\text{temperature}} *0.000716792 +
N317*1.00052
N317 = 1.04749
                     - temperature*0.00242951
temperature*concentration*0.001107
temperature^2*2.61671e-05 + concentration*0.0634356 -
concentration^2*0.00771838
N196 = 0.0184285 + N228*2.17991 + N228*N237*36.871
N228^2*19.2842 - N237*1.20936 - N237^2*17.5734
N237 = -0.807522 - N298*23.7389 + N298*N320*435.333 -
N298^2*207.154 + N320*26.1194 - N320^2*228.759
            93.1798
                      _
                            concentration*1.45848
concentration *N327*1.3814 - concentration ^2*0.00801795 -
N327*162.726 + N327^2*71.807
N327 = 1.0571 + \sqrt[3]{\text{temperature}} *0.0229108
N298 = 1.11674 - concentration^2*0.00218232
N321*1.04842 + N321^2*0.939285
N228 = -0.00598277 - N262*1.266 + N262^2*0.846248 +
N323*2.26972 - N323^2*0.845127
```

```
N323 = -1.2883e-09 + N324*1 \\ N324 = 0.230562 + concentration*11.0776 - concentration* \\ \hline{$\sqrt{\text{concentration}}$} *4.45051 + concentration^2*0.287269 + \\ \hline{$\sqrt{\text{concentration}}$} *4.72214 - "concentration, cubert"^2*10.763 \\ N262 = 4.13478 + \\ \hline{$\sqrt{\text{concentration}}$} *N321*1.13784 - N321*7.38699 + \\ N321^2*4.13226 \\ N321 = 1.52002 - \\ \hline{$\sqrt{\text{temperature}}$} *0.304285 + \\ \hline{$\sqrt{\text{temperature}}$} *2*0.0370877 - \\ \hline{$\sqrt{\text{concentration}}$} *0.233051 + \\ \hline{$\sqrt{\text{concentration}}$} ^2*0.0914517
```

### Appendix 3

```
N2 = -0.0439599 + \sqrt[3]{\text{temperature}} *0.0315586 - (
\sqrt{\text{temperature}} \(^2*0.00587683 + N3*1.00435\)
N3 = 0.155496 + N124*3.36364 + N124*N4*10.6424 -
N124^2*6.80354 - N4*2.66387 - N4^2*3.69322
N4 = 0.2407 + N133*0.592437 - N133*N6*11.8329 +
N133^2*5.52278 + N6^2*6.47899
N6 = 0.172566 - N105*2.66192 + N105*N10*6.1354 -
N105^2*1.84191 + N10*3.33287 - N10^2*4.13622
N10 = 0.0168257 - N23*1.5894 - N23*N18*209.588 +
N23^2*105.046 + N18*2.57135 + N18^2*104.542
N18 = -2.02643 - \sqrt[3]{concentration} / (*0.895731 + 
\sqrt[3]{concentration} *N20*0.954151 - (\sqrt[3]{concentration})
^2*0.0674471 + N20*5.58932 - N20^2*2.56794
N20 = -0.0169248 + N39*0.569435 + N64*0.44602
N39 = -0.539089 - N232*N71*0.472651 + N71*2.01153
N232 = 1.94648 + N247*33.6372 - N247*N248*28.0279 -
N248*36.0753 + N248^2*29.5401
N248 = 0.557289 - N264*N270*11.8467 + N264^2*6.17808
+ N270^2*6.11286
N247 = 0.549857 - N272*N264*12.3273 + N272^2*6.35166
+ N264^2*6.42436
N23 = -0.014425 + N36*0.593471 + N64*0.4197
N64 = -0.0937814 + N79*1.15177 + N79*N122*85.318 -
N79^2*42.6294 - N122^2*42.7439
N122 = 0.548532 + N261*N146*49.3484 - N261^2*24.8914
- N146^2*23.9979
N146 = -0.23137 - N182*N203*0.7618 + N182^2*0.61223 +
N203*1.37537
N203 = 2.09602 + N272*3.52473 + N272*N224*35.0648 -
N272^2*19.1706 - N224*6.42145 - N224^2*14.0823
N261 = -0.710208 + \sqrt[3]{\text{size}} *0.233925 - \sqrt[3]{\text{size}} *
N270*0.224983 + (\sqrt[3]{\text{size}})^2*0.00254334 + N270*1.65562
N79 = -0.0347346 + N102*0.62386 + N139*0.407856
N102 = 0.542353 + N273*N163*28.7982 - N273^2*14.7338
- N163^2*13.5996
N163 = 0.217553 - N224*N260*7.71021 + N224^2*4.12828
+ N260*0.60079 + N260^2*3.76162
N36 = -0.591883 - N216*N71*0.517506 + N71*2.10902
N71 = 0.551944 - N119*N139*11.075 + N119^2*5.74133 +
N139^2*5.7826
N139 = 1.55236 - N272*1.90194 + N272*N166*30.9343 -
N272^2*14.9265 - N166^2*14.6503
N166 = -8.82794 + N276*19.9028 + N276*N254*6.69713 -
N276^2*12.0441 - N254*3.55413 - N254^2*1.29918
N254 = 27.6859 + \sqrt[3]{concentration} *6.98392
\sqrt[3]{concentration} *N272*7.25464 + (\sqrt[3]{concentration})
^2*0.412021 - N272*56.9199 + N272^2*30.2604
```

```
N182^2*47.6807 - N188*12.1472 + N188^2*58.9018
N188 = 1.42085 - \sqrt[3]{\text{temperature}} * 0.588204
\sqrt[3]{\text{temperature}} *N260*0.467063 + (\sqrt[3]{\text{temperature}})
^2*0.0172111 - N260^2*0.21691
N182 = 29.0248 + \sqrt[3]{concentration} *8.76141
\sqrt[3]{concentration} * N270*9.09928 + (\sqrt[3]{concentration})
^2*0.521972 - N270*61.0681 + N270^2*33.0526
N216 = 0.546654 + N251*N255*0.481086 - N255*0.0274444
N255 = 0.289361 - \sqrt[3]{\text{temperature}} *0.371995 +
\sqrt[3]{\text{temperature}} *N264*0.246878 + (\sqrt[3]{\text{temperature}})
^2*0.0194641 + N264*1.46935 - N264^2*0.567788
N251 = 1.05743 - \sqrt[3]{temperature} *0.332809
temperature *N270*0.314313
N105 = -0.0935853 + N154*N249*105.233
N154^2*51.5875 + N249*1.18871 - N249^2*53.7343
N249 = 0.556159 - N265*N269*10.2422 + N265^2*5.3785 +
N269^2*5.30922
N269 = 0.5535 + N270^2*0.450366
N270 = 1.79649 - N272*N274*12.909 + N272^2*6.75012 -
N274*2.30547 + N274^2*7.67239
N265 = 8.05927 - N276*8.19174 + N276*N273*7.9282 -
N273*5.8934 - N273^2*0.87347
N154 = 0.042493 + N198*0.938548 - N198*N244*27.173 +
N198^2*13.4947 + N244^2*13.6932
N244 = 0.658433 + N260*2.99416 - N260*N264*2.12405 -
N264*3.20345 + N264^2*2.67723
N264 = 8.29568 - N274*6.43445 + N274*N276*7.84398 -
N274^2*0.586885 - N276*8.08886
N198 = 1.96822 + N276*6.0685 + N276*N262*9.18779 -
N276^2*7.08292 - N262*9.1697
N262 = 1.21061 - \sqrt[3]{temperature} *0.432062 +
\sqrt[3]{\text{temperature}} *N272*0.326664 + (\sqrt[3]{\text{temperature}})
^2*0 011487
N133 = 0.533045 + N271*N147*14.0159 - N271^2*7.13996
- N147^2*6.40515
N147 = 0.453799 - N204*2.8159 - N204*N212*61.038 +
N204^2*32.0004 + N212*3.04547 + N212^2*29.353
N212 = 1.21768 + N258^2*0.258996 - N260*1.25115 +
N260^2*0.778276
N258 = 3.26009 - \sqrt[3]{concentration} *2.51817 +
\sqrt[3]{concentration} *N276*2.41249 - N276*2.10711
N204 = 0.568517 + N224*6.03238 - N224*N256*4.76589 -
N256*6.1257 + N256^2*5.28845
N224 = 13.3683 - N272*13.3582 + N272*N276*14.1144 -
N272^2*0.530601 - N276*10.3193 - N276^2*2.19885
N276 = 0.355487 + \sqrt[3]{temperature}
\sqrt[3]{\text{temperature}} * \sqrt[3]{\text{size}} * 0.0486913 - (\sqrt[3]{\text{temperature}})
^2*0.0199388 + \sqrt[3]{\text{size}}*0.125759 + (\sqrt[3]{\text{size}})^2*0.00316425
N271 = -478.911 + N274*53.3607 - N274*N273*6916.64 +
N274^2*3042.39 + N273*819.436 + N273^2*3478.51
N124 = -0.517161 + N273*9.81491 + N273*N191*56.0058 -
N273^2*32.7723 - N191*7.89626 - N191^2*23.6331
N191 = 1.12128 - N256*3.66051 - N256*N260*1.89471 +
N256^2*2.86522 + N260*2.56987
N260 = 52.004 + \sqrt[3]{concentration} *15.6875
\sqrt[3]{concentration} *N274*16.3572 + (\sqrt[3]{concentration})
^2*1.04945 - N274*109.218 + N274^2*58.2556
N256 = 1.84353 - \sqrt[3]{\text{temperature}} *0.864108 +
\sqrt[3]{\text{temperature}} *N274*0.735576 + (\sqrt[3]{\text{temperature}})
^2*0.0157507 - N274^2*0.603494
```

N119 = 0.851494 + N182\*11.6096 - N182\*N188\*105.899 +

### Appendix 4

```
N23 = 0.00307904 - N277*0.305848 + N28*1.30313
N28 = -0.0226528 + N70*N91*8.4779 - N70^2*3.99666 +
N91*1.03745 - N91^2*4.49637
N91 = 0.0522123 + N125*4.7784 + N125*N212*3.597 -
N125^2*3.55704 - N212*3.86989
N212 = 0.177446 - N253*6.1007 + N253^2*3.25318 +
N387*6.80485 - N387^2*3.13152
N387 = 0.141524 - N444*3.39422 - N444*N459*3.10179 +
N444^2*3.20254 + N459*4.15331
N459 = -124.77 + \sqrt[3]{concentration} *0.0378238 +
\sqrt[3]{concentration} ^2*0.116687 + N491*222.531
N491^2*98.4561
N444 = -16.3901 + N460*N484*0.877107 + N484*29.7593 -
N484^2*13.4876
      = 1.04749 - temperature*0.00242951
temperature*concentration*0.001107
temperature^2*2.61671e-05 + concentration*0.0634356 -
concentration^2*0.00771838
N253 = 0.314215 + N336*3.73675 - N336*N410*23.1994 +
N336^2*10.372 - N410*3.2753 + N410^2*13.0539
N410 = -91.7218 - N462*N491*0.63044 + N462^2*0.758592
+ N491*163.368 - N491^2*71.9743
N491 = 1.47363 - \sqrt[3]{\text{size}} *0.268828 + \sqrt[3]{\text{size}} ^2 *0.0464843
N462 = 1.02129 - temperature*0.00394802 + temperature*
\sqrt[3]{concentration} *0.00316982 + temperature^2*2.19221e
05 + \sqrt[3]{concentration} ^2*0.0750819
N125 = 0.0593708 - \sqrt[3]{\text{temperature}} *0.0526818 +
temperature ^2*0.0103755 + N249*0.999156
N249 = 0.210198 - N340*3.14759 - N340*N467*15.9214 +
N340^2*9.94396 + N467*3.79125 + N467^2*6.12431
N340 = 5.7487 - N431*3.66406 + N431*N485*5.85338 -
N431^2*0.874882 - N485*6.0452
N70 = -0.151182 - N436*1.75082 + N436*N132*1.09555 +
N132*3.01942 - N132^2*1.21378
N132 = 0.111289 + N473*2.68781 - N473*N311*15.0922 +
N473^2*6.13742 - N311*1.84972 + N311^2*9.00755
N311 = 5.25361 - N422*3.29345 + N422*N478*5.52594 -
N422^2*0.875062 - N478*5.60742
N478 = 2.54991e-11 + N489*1
N422 = -0.104214 + N436*4.42879 - N436*N475*3.00016 -
N475*3.25346 + N475^2*2.92684
N473 = 1.95189 - \sqrt[3]{concentration} *2.21891 +
\sqrt{\text{concentration}} *N485*2.18895 - N485^2*0.859319
N12 = -0.122877 - N368^2*0.0946185 + N52*1.21636
N52 = -0.00143798 + N67*0.602684 + N99*0.398585
N99 = -0.0608305 + N379*5.19705 + N379*N141*30.2437 -
N379^2*17.5259 - N141*4.08064 - N141^2*12.7719
N141 = 0.023142 - N277*7.53984 - N277*N283*101.533 +
N277^2*54.1334 + N283*8.50377 + N283^2*47.4106
N283 = -0.0661891 - N345*4.98658 - N345*N355*26.189 +
N345^2*15.4951 + N355*6.11953 + N355^2*10.6263
N355 = 0.320408 - temperature*0.00863531
temperature*N431*0.00842796 + N431*0.686808
N431 = 1.74582
                     + concentration*0.0621551
                     ∛size
                                *0.0145533
concentration*
concentration^2*0.00384072 - \sqrt[3]{size}*0.636001 + - \sqrt[3]{size}
^2*0 116188
N345 = 5.68121 - N432*3.72705 + N432*N485*5.67002 -
```

```
N432^2*0.758563 - N485*5.84749
N277 = 0.254285 - N347*1.16728 - N347*N471*19.5149 +
N347^2*10.9315 + N471*1.74658 + N471^2*8.75207
N471 = 1.97737 - \sqrt[3]{concentration} *2.28187
\sqrt[3]{concentration} *N489*2.24388 - N489^2*0.878485
N347 = 5.86356 - N432*3.85011 + N432*N489*5.85103 -
N432^2*0.795616 - N489*6.04829
      =
             1.07598
                       + temperature*0.0025498
temperature*size*4.08789e-05
                              - size*0.00298495
size^2*6.64561e-05
                     - <sup>3</sup>√temperature *0.304285
N465 = 1.52002
                     <sup>3</sup>√concentration
                                         *0.0955142
 temperature
\sqrt[3]{\text{temperature}}^2 \cdot 2*0.0370877 - \sqrt[3]{\text{concentration}}*0.233051
+\sqrt[3]{concentration}^2*0.0914517
N282 = 0.0742453 + N342*4.14822 - N342*N428*2.86202 -
N428*3.28937 + N428^2*2.92798
N493 = 1.0571 + \sqrt[3]{\text{temperature}} *0.0229108
           0.433692 - temperature*0.0128194
temperature*N475*0.0112107 + temperature^2*1.65897e-05
+ N475*0.597218
N342 = 5.96116 - N436*3.81995 + N436*N484*6.04972 -
N436^2*0.904905 - N484*6.26513
N169 = 0.501787 - concentration^2*0.0026461 +
N282^2*0.497111
N475 = 0.230562 + concentration*11.0776 - concentration
* \sqrt[3]{concentration} *4.45051 + concentration^2*0.287269 +
\sqrt[3]{concentration}*4.72214 - \sqrt[3]{concentration}^2*10.763
N67 = -0.0966324 + N120*5.34773 + N120*N169*3.91114
N120^2*3.97676 - N169*4.18742
N379 = 0.0576154 + N432*6.46599 - N432^2*2.52785 -
N465*5.58326 + N465^2*2.58636
N484 = 0.896649 - size^{*3} \sqrt{temperature} *0.0013362 +
size^2*6.55798e-05 + \sqrt[3]{temperature}*0.0825952
N120 = 25.9835 - N492*45.579 + N492*N250*0.880739 +
N492^2*19.9874
N250 = 0.201532 - N336*3.01893 - N336*N467*15.9805 +
N336^2*9.90949 + N467*3.67825 + N467^2*6.21086
                       - concentration*0.554298
            -19 8242
concentration*N488*0.590246 - concentration^2*0.0116462
+ N488*37.0513 - N488^2*16.4755
N488 = 1.1946 + temperature*0.00396623 - temperature*
\sqrt[3]{\text{size}} *0.000954049 - \sqrt[3]{\text{size}} *0.121022 + \sqrt[3]{\text{size}}
^2*0.0258324
N336 = 5.71918 - N436*3.63394 + N436*N485*5.84165 -
N436^2*0.882014 - N485*6.02784
N485 = 0.836083 + \sqrt[3]{\text{temperature}} *0.135803 -
\sqrt[3]{\text{temperature}} * \sqrt[3]{\text{size}} * 0.0330707 + \sqrt[3]{\text{size}}^2 * 0.0173862
N436 = 1.0698 + concentration*0.0830254
concentration*size*0.000639263
concentration^2*0.00367463
                                     size*0.015615
size^2*0.000268299
N492 = 0.538778 + \sqrt[3]{\text{temperature}} *0.0116771
N493*0.490323
N368 = 0.961219 - \sqrt[3]{\text{temperature}} *0.33494
₹ temperature *N432*0.249184
^2*0.0125925 + N432*0.181389
  (1) N432 = 1.09013 - size*0.0161022 + size*
\sqrt{concentration} *0.00166551 + size^2 *0.000260082 -
\sqrt[3]{concentration}*0.115233 + \sqrt[3]{concentration}*0.173351
```