2011 2nd International Conference on Biotechnology and Food Science
IPCBEE vol.7 (2011) © (2011) IACSIT Press, Singapore

Software packages for food engineering needs

Abakarov, A.
Universidad Politécnica de Madrid
Madrid, Spain.
e-mail: alik.abakarov@usm.cl

Abstract — **The graphic user interface (GUI) software packages "ANNEKs" and "OPT-PROx" are developed to meet food engineering needs. "OPT-RROx" (OPTimal PROfile) is software developed to carry out thermal food processing optimization based on the variable retort temperature processing and global optimization technique. "ANNEKs" (Artificial Neural Network Enzyme Kinetics) is software designed for determining the kinetics of enzyme hydrolysis of protein at different initial reaction parameters based on the Artificial Neural Network's and adaptive random search algorithm. The "OPT-PROx" software was successfully tested on the real thermal food processing problems, and has demonstrated a significant advantage over the traditionally used constant temperature processes in terms of total processing time and final product quality. The "ANNEKs" software can be effectively used for process design of enzyme hydrolysis of protein. The proposed in this research user friendly dialogue software can be useful for food scientists and engineers.**

Keywords - sophisticated software; thermal food processing; enzyme kinetics; artificial neural networks; adaptive random search.

I. INTRODUCTION

Food engineering is the multidisciplinary field of applied sciences combined with the knowledge of product properties [1]. Food engineers provide the technological knowledge transfer essential to the cost-effective production and commercialization of food products and services. In the development of food engineering, one of the many challenges is to employ state-of-art mathematical methods and based on these methods sophisticated dialogue software to develop new products and processes.

It is well-known, that the thermal processing of canned foods and enzymatic hydrolysis of food proteins are typical topics of food engineering [1, 2]. These topics are of great interest due to their numerous applications and potential economic importance [1, 2, 3].

Thermal processing is one of the most important industrial technologies of food preservation in the manufacture of shelf stable canned foods [4]. Mainly, thermal processing is concentrated on the following factors: final product safety and quality, total processing time and energy consumption. The diversity of thermal processing objectives impose different optimal requirements to sterilization processing, which can be determined analytically or by numerical procedures and based on these procedures sophisticated dialogue software.

Enzymatic hydrolysis of food proteins is well-known method to modify and improve their functional and nutritional properties [2, 3]. It provides desirable characteristics from the food technology point of view. Protein hydrolysates are typically employed as food ingredients to stabilize interfaces, bind water, lipids and aroma, solubilise other ingredients or improve organoleptic features of the product such as colour, odour and flavor [2, 3]. It is known that the protein structure is sensitive to processing conditions. Therefore, in approaching the process design for the enzyme hydrolysis of proteins, it is important to be able to predict processing outputs in response to different input variables, such as substrate and enzyme initial concentrations, and hydrolysis time. A useful tool for this purpose is an accurate mathematical model, however, in many cases it is difficult to construct a proper model for an enzymatic reaction since the constructed kinetic model obeys an enzyme with reaction conditions in which the kinetic constants were estimated only. At the same time, the determination of kinetic constants for other required reaction conditions could be extremely difficult due to their time consuming procedures and cost. An alternative approach to obtaining a model of the reaction kinetics would be the use of Artificial Neural Networks (ANNs), since it is well known that ANNs can work as universal approximator of non-linear functions and, basing on the experimental data, can be successfully used in assessing the dynamics of complex processes.

Well designed dialogue software significantly simplifies an engineering calculations process from its initial stage consisted of problem definition or (and) parameterization to the final stage consisted of realizing required computations. Thus, the objective of this research consisted of development graphic user interface (GUI) software packages to meet such food engineering needs as thermal food processing optimization and determining the kinetics of enzyme hydrolysis of protein at different initial reaction parameters

II. METHODS

Problem statement for thermal sterilization of canned foods

In the particular case of a cylindrical container with radius R and height $2L$, the mathematical model describing heat transfer by conduction is a mixed boundary problem, as follows [1]:

$$\frac{\partial T}{\partial t} = \alpha\left(\frac{\partial^2 T}{\partial r^2} + \frac{1}{r}\frac{\partial T}{\partial r} + \frac{\partial^2 T}{\partial z^2}\right),$$

where T is temperature, t is time, r and z are radial and vertical locations within the container, and alpha (α) is the thermal diffusivity of the product.

The model has the following initial and boundary conditions (by symmetry):

$$T(R,z,t) = T_{rt}(t),\ T(r,L,t) = T_{rt}(t),\ \frac{\partial T}{\partial r}(0,z,t) = 0,$$

$$\frac{\partial T}{\partial z}(r,0,t) = 0,\ T(r,z,0) = T_{in},$$

where $T_{rt}(t)$, $t \in \left[0, t_f\right]$ will be the retort temperature as a function of time, and T_{in} is the initial temperature at $t = 0$. The lethality constraint can be specified as follows: i) $F_0(t_f) \geq F_0^d$, where F_0^d is the final required lethality and is calculated according to the following equation:

$$F_0(t) = \int_0^{t_f} 10^{\frac{(T-T_{ref})}{z}} dt ,$$

Where T is the temperature at the critical point or cold spot, and T_{ref} is the reference temperature.

Quality retention is greatly affected by the non-uniform temperature distribution within the package from the heated boundary to the cold spot, and it must be integrated in space over the volume of the container as well as over time. To accomplish this integration over both space and time, the following approach was used:

ii) $\overline{C(t_f)} \geq C^d$, where C^d is the desired volume-average final quality retention value and is calculated as shown in the following equation:

$$\overline{C(t)} = C_0 \frac{2}{LR^2} \int_0^L \int_0^R \exp\left[-\frac{\ln 10}{D_{ref}} \int_0^{t_f} 10^{\frac{(T-T_{ref})}{z}}\right] dr dz$$

The following types of single thermal process optimization problems were considered over the last few decades [5]:

1. Find such a retort function, where the final quality retention is maximized, while the final process lethality is held to a specified minimum.
2. Find a retort function, such that the total processing time is minimized subject to the same lethality requirement above, while the quality retention must not fall beneath some specified minimum;
3. Find a retort function, such that the final process time is minimized subject to the same lethality requirement above, while the quality retention must not fall beneath some specified minimum, and energy consumption must not exceed a specified maximum; minimum and maximum values are computed at constant retort temperature profiles.

In the general case, the retort function $T_{rt}(t)$ over $t \in [0 : t_f]$ can be parameterized using N_p points, and during each time interval $t_k' = [t_k, t_{k+1})$, $k \in 0 : (N_p - 1)$, the value of $T_{rt}(t_k')$ remains constant at u_k [6]. However, in this case, the use of a cubic spline in approaching global optimization problems with random search techniques can produce superior results over discrete step-wise functions [7], mainly because the cubic spline approximation allows for significantly reducing the number of decision variables and therefore the necessary number of objective function computations to reach the global solution. Therefore, the cubic spline approximation coupled with adaptive random search algorithm [5, 7] are utilized in this study in order to find optimal variable retort temperature (VRT) profiles.

Exponential kinetic equation

The following well-known exponential kinetic equation presents a relationship between the reaction rate R, and the concentrations of initial substrate S_0 and enzyme E_0 [8]:

$$\frac{dDH}{dt} = a \exp(-bDH)$$

where the coefficients a and b have different expressions according to different reaction mechanisms. For example, the following expressions of coefficients a and b can be used for the mechanism of substrate-inhibition:

$$a = \frac{k_2 k_s E_0}{S_0 k_s + S_0^2} \qquad b = \frac{k_3 k_m k_s}{k_2 \left(k_s + S_0\right)} \qquad k_3 = \frac{k_m}{k_d}$$

where: k_m is M-M constant, k_s is a substrate inhibition constant, k_2 is a reaction rate constant of enzymatic hydrolysis, k_d is a inactivation constant of enzyme.

Determination of the kinetics of enzyme hydrolysis

The two following approaches are used in this study for determining the kinetics of enzyme hydrolysis of protein at different initial reaction parameters:

1. This approach consists of estimating the parameters of exponential kinetic equation. The best-fitting parameters (for example, kinetic constants k_m, k_s, k_2 , k_d) are estimated from time course profiles (TCPs) as a regression problem. Namely, an adaptive random search algorithm is used to minimize the sum of squared residuals. Use of this method can give much greater confidence than if a true global optimal solution had existed within the global domain (better than local optima), since then it would not have been missed by the search routine.
2. This approach consists of using the ANNs for estimating the coefficients a and b of exponential kinetic equation. In this approach each of the experimental TCPs are fitted to exponential equation by an adaptive random search technique. Obtained optimal a and b values obtained for TCPs, and different initial reaction parameters (for example, initial enzyme and substrate concentrations) are used as a given and (input) data for the ANNs learning process.

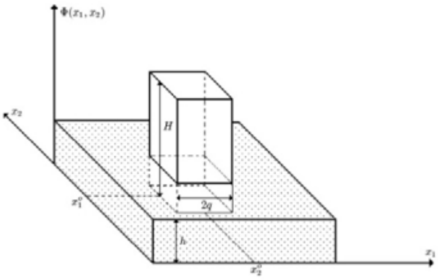


Figure 1. Pedestal frequency distribution for a two-dimension case.

Adaptive random search algorithm

The adaptive random search algorithm belongs to a specific class of global stochastic optimization algorithms [8]. This class of algorithms is based on generating the decision variables from a given probability distribution, and the term ‘‘adaptive” consists of modifications to the probability distribution utilized in the searching process, which, throughout the whole search process, act as minimum computations of the objective function, locating global solutions. The pedestal probability distribution is utilized in the adaptive random search. After every calculation of objective function, the pedestal distribution of decision variables is modified so that the probability of finding the optimal value of the objective function is increased. For example, Fig. 1 shows a pedestal frequency distribution for the two-dimensional case of an optimization problem can be obtained in the middle of the search process.

III. RESULTS

“OPT-PROx” software

Borland C++ Builder 6.0 was used to create the “OPT-PROx” software [7, 12]. “OPT-PROx” software contains two worksheets oriented to the numerical determination of heat transfer coefficient (Fig. 2) and thermal food processing optimization (Fig. 3).

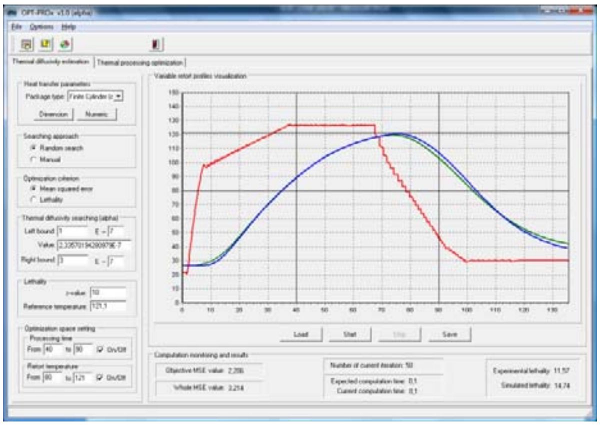


Figure 2. Worksheet for determination of heat transfer coefficient.

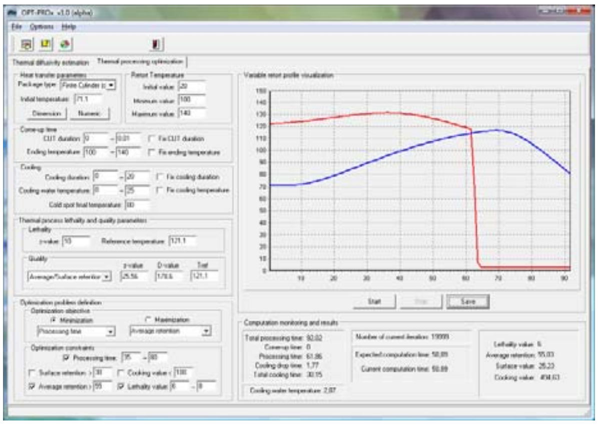
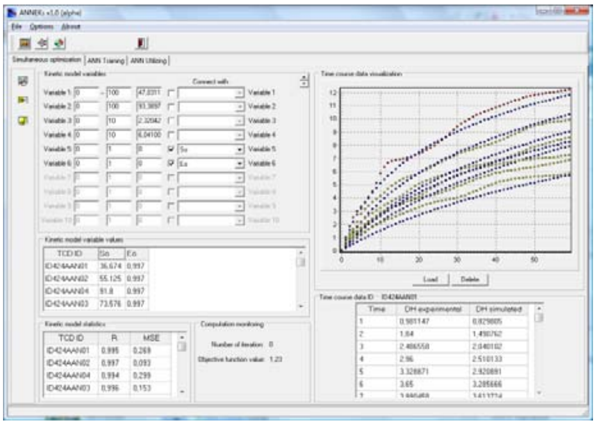


Figure 3. Thermal food processing optimization worksheet.

The diversity of thermal food processing optimization problems with different objectives and required constraints are solvable by “OPT-PROx” package. The adaptive random search algorithm coupled with penalty functions approach, and the finite difference method with cubic spline approximation are utilized by “OPT-PROx” for simulation and optimization of the thermal food processes [5]. The mean square error minimization principle is utilized in order to estimate the heat transfer coefficient of food to be processed under optimal condition. The following types of objective functions and constraints are supported by “OPT-PROx” software. Types of objective functions: 1) minimization of total processing time, 2) minimization of cooking value, 3) maximization of aurface quality retention, 4) maximization of average quality retention. Optimization constraints for: 1) surface quality retention, 2) average quality retention, 3) cooking value, 4) thermal lethality value, 5) total thermal processing time. “OPT-PROx” GUI’s allows formulating a required optimization problem combining the mentioned above optimization objectives and constraints (Fig. 3).

Minimization processing time problem

This numerical experiment deals with searching for the optimum VRT profile to minimize processing time within the constraints of assuring both minimum required target lethality and quality retention [7]. In this case, the search routine was restricted in two ways, first to satisfy the lethality constraint of $F_0^{z} = 8$ minutes, and secondly that the quality thiamine retention could not fall below 55%, in other word the objective consisted of obtaining the product of better quality for minimal processing time is chosen. The optimum CRT process that will deliver minimum processing time while holding thiamine retention equal to 53% is a process with constant retort temperature at 118 °C and a process time of 98 minutes [7]. The result obtained by “OPT-PROx” software is shown in Fig. 3. In this case, the thiamine retention of 55% was achieved with a further reduction in processing time down to 62 minutes.



Variable 1: 0 – 100, 47.0311
Variable 2: 0, 100, 93.3897
Variable 3: 0, 10, 2.32042
Variable 4: 0, 10, 6.04100
Variable 5: 0, 1, 0, ☑ So
Variable 6: 0, 1, 0, ☑ Eo

Kinetic model variable values

TCD ID	So	Eo
ID424AAN01	36.674	0.997
ID424AAN02	55.125	0.997
ID424AAN04	91.8	0.997
ID424AAN03	73.576	0.997

Kinetic model statistics

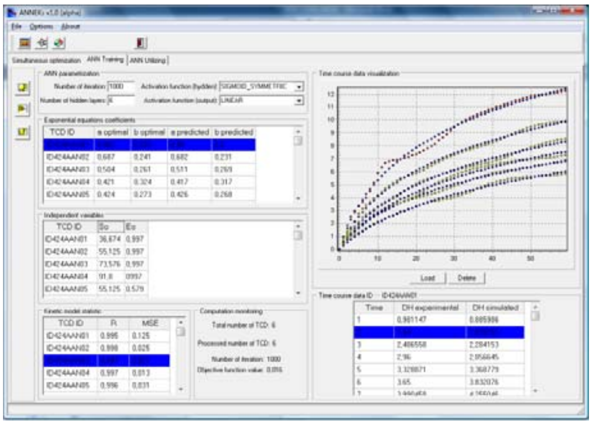
TCD ID	R	MSE
ID424AAN01	0.995	0.269
ID424AAN02	0.997	0.093
ID424AAN04	0.994	0.299
ID424AAN03	0.996	0.153

Computation monitoring
Number of iteration: 0
Objective function value: 1.23

Time course data ID: ID424AAN01

Time	DH experimental	DH simulated
1	0.981147	0.829805
2	1.84	1.490762
3	2.486558	2.040102
4	2.96	2.510133
5	3.328871	2.920891
6	3.65	3.285666

Figure 4. Simultaneous optimization worksheet.



ANN parametrization
Number of iteration: 1000
Number of hidden layers: 6
Activation function (hydden): SIGMOID_SYMMETRIC
Activation function (output): LINEAR

Exponential equations coefficients

TCD ID	a optimal	b optimal	a predicted	b predicted
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
ID424AAN02	0.687	0.241	0.682	0.231
ID424AAN03	0.504	0.261	0.511	0.269
ID424AAN04	0.421	0.324	0.417	0.317
ID424AAN05	0.424	0.273	0.426	0.268

Independent variables

TCD ID	So	Eo
ID424AAN01	36.674	0.997
ID424AAN02	55.125	0.997
ID424AAN03	73.576	0.997
ID424AAN04	91.8	0997
ID424AAN05	55.125	0.579

Kinetic model statistic

TCD ID	R	MSE
ID424AAN01	0.995	0.125
ID424AAN02	0.998	0.025
[illegible]	[illegible]	[illegible]
ID424AAN04	0.997	0.013
ID424AAN05	0.996	0.031

Computation monitoring
Total number of TCD: 6
Processed number of TCD: 6
Number of iteration: 1000
Objective function value: 0.016

Time course data ID: ID424AAN01

Time	DH experimental	DH simulated
1	0.981147	0.885986
[illegible]	[illegible]	[illegible]
3	2.486558	2.284153
4	2.96	2.956645
5	3.328871	3.368779
6	3.65	3.832076

Figure 5. Worksheets “ANN Training” and “ANN Utilizing”.

The “OPT-PROx” software was successfully tested on the real thermal food processing problems, and has demonstrated a significant advantage over the traditionally used constant temperature processes in terms of total processing time and final product quality [5, 7].

“ANNEKs” software

Borland C++ Builder 6.0 was used to design the “ANNEKs” software. “ANNEKs” contains three worksheets oriented to: a) estimating the kinetic parameters of exponential kinetic equation (Fig. 4), b) using the ANNs for estimating the coefficients *a* and *b* of exponential kinetic equation (Fig. 5). The worksheet “Simultaneous optimization” presents the following functionality: definition of number, bounds and initial values of variables used in the exponential kinetic equation (1); use the mathematical expression parser to define expressions for coefficients *a* and *b* according to the required reaction mechanisms; input of the experimental TCPs from text files and its graphical representation; computation of the MSE-values and Pearson correlation coefficients for each of the TCPs; adaptive random search algorithm parameterization. The “ANNEKs” software can be effectively used for process design of enzyme hydrolysis of protein [10, 11].

Estimation of a and b coefficients by “ANNEKs” software

Six experimental TCPs in the form of degree of hydrolysis over reaction time divided into two groups are shown in Fig. 6 [10, 11]. The first group consisted of TCPs for use in the training, and the second group consisted of TCPs used for testing model performance. The optimal values of coefficients *a* and *b* computed by “ANNEKs” for TCPs of both groups are presented in Table 1. Fig. 7 depicts the TCPs of both groups: training and testing along with the smooth curves corresponding to the optimal values of coefficients *a* and *b* from Table 1. The TCPs used for testing are shown in Fig. 8, along with the two smooth curves corresponding to the *a* and *b* values predicted by the ANN model. Table 3 summarizes information about the correlation coefficients and MSE values between the experimental TCPs and the curves obtained from the trained ANN-based model. The results obtained from ANNs approach realized by “ANNEKs” software indicate its high predictive performance for processes involving complex reaction kinetics.

IV. CONCLUSIONS

Findings from the work reported in this study would suggest that the developed user-friendly interfaces and utilized numerical approaches make the “OPT-PROx” and “ANNEKs” software packages useful for food scientists and engineers.

ACKNOWLEDGMENT

The author wishes to thank Dr. Sergio Almonacid and Dr. Ricardo Simpson, Department of Chemical and Environmental Engineering, Santa Maria Technical University, Chile, for collaboration related to the thermal food processing simulation and optimization, and modeling of food protein hydrolysis kinetic, which gave the additional opportunities to create the “OPT-PROx” and “ANNEKs” software packages.

REFERENCES

[1] F. Erdoğdu, “Optimization in food engineering,” CRC Press, New York, USA, 2009, 758 p.

[2] A. P. Urwaye, “New food engineering research trends”, Nova Science Publishers, Inc. New York, USA, 2008, 298.

[3] S. S. Nielsen, “Food Analysis” , Springer, New York, USA, 2010, 550 p.

[4] A. A. Teixeira, “Thermal process calculations”. In D. R. Heldman & D. B. Lund (Eds.), Handbook of food engineering, 1992 (pp. 563–619). New York: Marcel Dekker, Inc.

[5] A. Abakarov, Yu. Sushkov, S, Almonacid, R. Simpson, “Multi-objective optimization based on adaptive random search method: optimization of food processing”, Journal of Food Science, 2009, 74(9), E471 - E487.

[6] J. R. Banga, R. I. Perez-Martin, J. M. Gallardo and J. J. Casares, “Optimization of thermal processing of conduction-heated canned foods: Study of several objective functions. Journal of Food Engineering”, 1991, 14, 25–51.

[7] A. Abakarov, Yu. Sushkov, S. Almonacid and R. Simpson. “Thermal processing optimization through a modified adaptive random search”, Journal of Food Engineering, 2009, 93(2), 200-209.

[8] Q. Wei and H. Zhimin, “Enzymatic hydrolysis of protein: mechanism and kinetic model”, Front. Chem. China, 2006, 3: 308-314.

[9] A. Zhigljavsky and A. G. Zilinskas, “Stochastic Global Optimization. Ser. Springer Optimization and Its Applications”, vol. 9. Springer-Verlag, Berlin, 2008, xvi+362 p. ISBN:0-387-36720-0.

[10] S. Almonacid, A. Abakarov, R. Simpson, P. Chávez, and A. Teixeira, “Estimating reaction rates in squid protein hydrolysis using artificial neural network”, Journal Transactions of the ASABE, 2009, 52(6), 1969-1977.

[11] A. Abakarov, A. Teixeira, R. Simpson, M. Pinto, and S. Almonacid. “Modelling of squid protein hydrolysis: Artificial Neural Network approach”. Journal of Food Process Engineering. DOI: 10.1111/j.1745-4530.2009.00567. 2010.

[12] Abakarov A. ToMakeChoice. 25 Oct. 2010. <http://tomakechoice.com/optprox/>

TABLE 1. OPTIMAL VALUES OF COEFFICIENTS A AND B.

	Initial substrate and enzyme concentrations (g/L)					
	TCPs of learning group				TCPs of testing group	
So	36.67	55.13	55.13	91.8	73.58	55.13
Eo	0.997	0.997	0.298	0.997	0.997	0.597
a	0.939	0.658	0.284	0.437	0.509	0.425
b	0.197	0.235	0.308	0.331	0.264	0.273

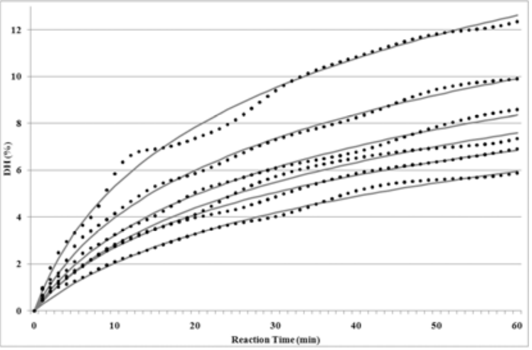


Figure 6. Six experimental TCPs divided into two groups.

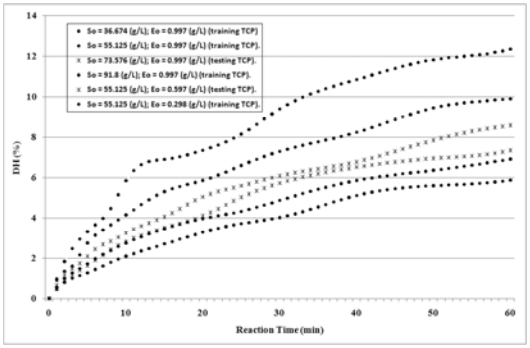


Figure 7. TCPs used for testing along with the smooth curves

TABLE 3. CORRELATION COEFFICIENTS AND MSE VALUES BETWEEN EXPERIMENTAL AND PREDICTED CURVES

	Initial substrate and enzyme concentrations (g/L)					
	TCPs of learning group				TCPs of testing group	
So	36.67	55.13	55.13	91.8	73.58	55.13
Eo	0.997	0.997	0.298	0.997	0.997	0.597
R^2	0.996	0.998	0.997	0.997	0.997	0.996
MSE	0.0938	0.0267	0.0185	0.0152	0.0309	0.0329

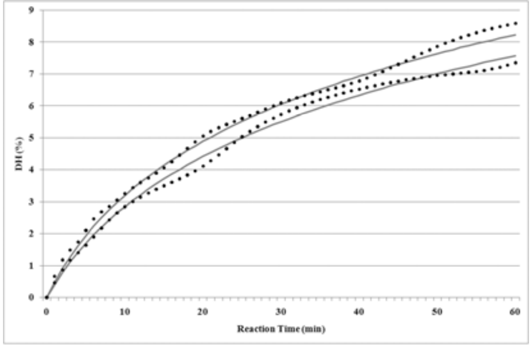


Figure 8. TCPs used for testing along with the smooth curves predicted by “ANNEKs” software package.