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PREFERENCES AND DETERMINATION OF THE NOMINAL GROWTH RATE OF FED-BATCH PROCESS: CONTROL DESIGN OF COMPLEX PROCESSES

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Keywords: Expected utility, machine learning, preferences, complex process, optimal control, Monod kinetic, growth rate

1. Introduction

The specific growth rate of the fed-batch processes determines the nominal biotechnological condition [14, 16]. The complexity of the biotechnological fermentation process makes difficult the determination of the *"best"* process parameters. The incomplete information sometimes is compensated by the use of imprecise human estimations [8, 12, 13]. People's preferences contain characteristics of subjective and probabilistic uncertainty. This makes difficult the mathematical incorporation of human preferences in complex systems. The necessity of a merger of empirical knowledge with mathematical exactness and descriptions causes difficulties. Possible approach for solution of these problems is the stochastic approximation ([1, 4, 5]). The uncertainty of the subjective preferences could be viewed as a noise which can be eliminated as typical for the stochastic approximation procedures. A main requirement of the stochastic assessment is the analytical presentation of the qualitative nature of the human's preferences and notions ([1, 12, 18]).

Our experience is that the human estimation of the process parameters of a cultivation process contains uncertainty in the range from 10% to 30%. Here a mathematical utility evaluation procedure for elimination of the uncertainty in the decision-maker's (DM) preferences and evaluation of the DM's utility is proposed [1, 12, 15, 18]. The approach permits iterative and precise evaluation of the *"best"* growth rate of the fed-batch process in agreement with the DM's preferences as maximum of this utility function [15]. In the paper is presented

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mathematical methodology that is useful for dealing with the uncertainty of human behavior and judgment in complex control problems and mathematical description of the complex system *"technologist-fed-batch process"* . The dialogue *"DM - computer"* realizes a machine learning on the base of the DMs preferences.

2. Description of fed-batch extended Monod kinetic model

Mathematical unstructured models of fed-batch process can be written based on mass balance equations [14, 19, 20]. Unstructured models take cell mass as a uniform quality without internal dynamic. The reaction rates depend only upon the macroscopic conditions in the liquid phase of the bioreactor. Below we investigate an extended form Wang-Monod model [20]. In Monod kinetic model the acetate and the ethanol production are included [16, 19, 20]. In the case of *E-coli* cultivation the equation describing the ethanol production can be omitted. The dynamics of the specific growth rate in the modification proposed by Wang in Wang-Monod model is described as a first order lag process with a rate constant in response to the deviation in the growth rate [20]:

$$
\begin{aligned}
\dot{X} &= \mu X - \frac{F}{V}X, \\
\dot{S} &= -k\mu X + (S_0 - S)\frac{F}{V}, \\
\dot{\mu} &= m\left(\mu_m \frac{S}{(K_S + S)} - \mu\right), \\
\dot{V} &= F, \\
\dot{E} &= k_2\mu E - \frac{F}{V}E, \\
\dot{A} &= k_3\mu X - \frac{F}{V}A,
\end{aligned} \tag{1}
$$

where X is the concentration of biomass, [g/l]; S - the concentration of substrate (glucose), [g/l]; V - bioreactor volume, [l]; F- substrate feed rate (control input), [h^{-1}]; S_0 - substrate concentration in the feed, [g/l]; μ_{max}- maximum specific growth rate, [h^{-1}]; K_S - saturation constant, [g/l]; k, k_2 and k_3 - constants, [g/g]; m-coefficient [-]; E- the concentration of ethanol, [g/l]; A - the concentration of actate, [g/l]. We preserve the notation $U(\cdot)$ fot the criteria for optimization (*a unimodal polynomial utility functionof degree 6 in this investigation*[15, 16]. The system parameters are as follows: $\mu_m = 0.59[\mathrm{h}^{-1}]$, $K_S = 0.045$ [g/l], $m = 3$ [-], $S_0 = 100$ [g/l], $k_2 = 3.79$ [-], $k_3 = 1/71$ [-], $k_E = 50$ [-], $F_{max} = 0.59$ [h^{-1}], $V_{max} = 1$ [l]. The 5^{th} equation describes the production of ethanol *(E)*. The last equation describes the production of acetate *(A)*. This equation is dynamically equivalent to the first one after the implementation of a simple transformation ($X = (1/k_3)A$). The initial state variables are taken as follows:

$$X_i(0) = 0.99; S_i(0) = 0.01; \mu_i(0) = 0.1; E_I(0) = 0.01; V_i(0) = 0.5.$$

3. Value and Utility Functions

We begin with the simplest case, the value functions ([8, 12]). Let $\mathbf{X}$ be the set of alternatives ($\mathbf{X} \subseteq \mathbf{R^m}$). A "value" function is a function $u^*(\cdot)$ for which it is fulfilled (Keeney & Raiffa, 1976):

$$((x, y) \in \mathbf{X^2}, x \succ y) \Leftrightarrow (u^*(x) > u^*(y)) \tag{2}$$

The decision maker's (DM's) preferences over X are expressed by ($\succ$). A value function gives us only the possibilities for determination of the maximum or minimum of a solution. The analytical presentation of a value function could be used in optimal control problem for description and control of complex dynamical biotechnological problems. Mathematical expectations with value functions are not possible. The description of a utility function is more difficult. Let $\mathbf{X}$ be a set of alternatives and $\mathbf{P}$ is a subset of discrete probability distributions over $\mathbf{X}$. A utility function is any function $u(\cdot)$ for which it is fulfilled ([8]):

$$\left(p \succ q,\ (p, q) \in \mathbf{P^2}\right) \Leftrightarrow \left(\left(\int u(\cdot)\ dp > \int u(\cdot)\ dq\right),\ p \in \mathbf{P},\ q \in \mathbf{P}\right) \tag{3}$$

According to Von Neumann and Morgenstern the above formula means that the mathematical expectation of $u(\cdot)$ is a quantitative measure in the interval scale with regard to the expert's preferences for probability distributions $\mathbf{P}$ over $\mathbf{X}$ ([8, 12, 18]). The DM's preferences over $\mathbf{P}$, including those over $\mathbf{X}$, ($\mathbf{X} \subseteq \mathbf{P}$) are expressed by($\succ$). The indifference realtion $\sim$ is defined as

$$((x \sim y) \Leftrightarrow \neg((x \succ y) \vee (x \prec y)))\,.$$

It is well known that the existence of an utility function $u(\cdot)$ over $\mathbf{X}$ determines the "preference" relaton ($\succ$) as a as a negatively transitive and asymmetric one ([8])

Proposition 1. *If the relation ($\succ$) is negatively transitive and asymmetric, the "indifferenece" relation ($\sim$) is transitive.*

Corollary 1. *If the relation ($\succ$) is negatively transitive and reflexive, the "indifferenece" relation ($\sim$) is an "equivalence" [8] .*

Every discrete probability distribution over $\mathbf{X}$ is called a "lottery". We denote the lottery as $\langle x, y, \alpha\rangle$ where α is the probability of the appearance of the alternative x and $(1-\alpha)$- the probability of the alternative y. The most used approach in assessment of the utility uses the following comparisons: $z \sim \langle x, y, \alpha\rangle$, where $(x \succ z \succ y)$, $\alpha \in [0, 1]$, $(x, y, z) \in \mathbf{X^3}$ ([7, 12, 18]). The weak points of these approaches are the so called "certainty effect" and "probability distortion" identified by Kahneman and Tversky ([10, 11, 13]). The determination of the best alternative x and the worst alternative y on condition that $(x \succ y \succ z)$ where z is the analyzed alternative is not easy. The transitivity violations of the "indifference" relation lead to the declinations in the assessments (Cohen, & Jaffray, 1988). They explain the DM behaviour observed in the famous Allais Paradox that arises from the "independence" axiom ([8]):

$$\big(p \succ q, 0 < \alpha < 1, (p, q, r) \in \mathbf{P^3}\big) \Rightarrow ((\alpha p + (1 - \alpha)r) \succ (\alpha q + (1 - \alpha)r)) \quad (4)$$

The utility function $u(\cdot)$ over $\mathbf{X}$ is determined with the accuracy of the affine transformation (interval scale), according to the following proposition ([8]):

Proposition 2. *If* $(x \in X, ((p(x) = 1) \Rightarrow (p \in \mathbf{P})))$ *and* $((q, p) \in \mathbf{P^2} \Rightarrow \alpha p + (1 - \alpha q) \in P, \alpha \in [0, 1])$ *are realized, then* $u(\cdot)$ *is defined with precision up to the affine transformation* $(u_1(\cdot) \sim u_2(\cdot)) \Leftrightarrow (u_1(\cdot) = au_2(\cdot)+b, a > 0 \wedge b \in \mathbf{R})$.

This property is essential for the application of the utility theory, since it allows a decomposition of the multiattribute utility functions into simpler functions [12]. The first condition in Proposition 2 can be interpreted as a capability of the DM to imagine one alternative independently on the others. The second condition is a capability of the DM to report on the uncertainty of the results. This proposition reveals that the utility measurement scale of the utility function is equivalent to the temperature scale (interval scale). Several non-expected utility theories have been developed in response of the displayed transitivity violations [10, 11, 13]. Among these theories the rank dependent utility model and its derivative cumulative prospect theory are currently the most popular. In the rank dependents utility (RDU) the decision weight of an outcome is not just the probability associated with this outcome. It is a function of both the probability and the rank (the alternative) x. For example the RDU of the lottery $(p_1, x_1; p_2, x_2; \ldots; p_n, x_n)$ is:

$$RDU = \sum_{i=1}^{n} W(p_i)u(x_i).$$

Based on empirical researches several authors have argued that the probability weighting function $W(\cdot)$ has inverse S-shaped form, which starts on concave and then becomes convex. Our approach permits accounting for this particular case and evaluations in the conceptions of RDU.

4. Utility evaluation and stochastic approximation

The following notations will be used:

$$\begin{aligned} A_u &= \{(\alpha, x, y, z) |\ \alpha u(x) + (1 - \alpha)u(y) > u(z)\}\,; \\ B_u &= \{(\alpha, x, y, z) |\ \alpha u(x) + (1 - \alpha)u(y) < u(z)\} \end{aligned} \quad (5)$$

The expected DM utility is constructed by pattern-recognition of A_u and B_u [1, 15]. Key element in this solution is the next proposition [15]:

Proposition 3. *If* $A_{u_1} = A_{u_2}$ *then* $u_1(\cdot) = au_2(\cdot) + b, a > 0$.

The following presents the procedure for evaluation of the utility functions:
The DM compares the "lottery" $\langle x, y, \alpha \rangle$ *with the simple alternative* $\mathbf{z}, \mathbf{z} \in \mathbf{X}$ *("**better** -* $\succ$*,* $\mathbf{f(x,y,z,}\boldsymbol{\alpha}\mathbf{) = 1}$*", "worse -* $\prec$ *,* $\mathbf{f(x,y,z,}\boldsymbol{\alpha}\mathbf{) = -1}$*" or "can not answer or equivalent -* $\sim$*,* $\mathbf{f(x,y,z,}\boldsymbol{\alpha}\mathbf{) = 0}$*",* $f(\cdot)$ *denotes the qualitative DM answer). This determines a learning point* $((\mathbf{x,y,z,}\boldsymbol{\alpha}), \mathbf{f(x,y,z,}\boldsymbol{\alpha}\mathbf{)})$*. The following recurrent stochastic algorithm constructs the utility polynomial approximation* $u(x) = \sum_i \Phi_i(x)$

$$\begin{aligned} c_i^{n+1} &= c_i^n + \gamma_n \left[f(t^{n+1}) - \overline{(c^n, \psi(t^{n+1}))} \psi_i(t^{n+1}) \right] \\ \sum_n \gamma_n &= +\infty, \sum_n \gamma_n^2 < +\infty, \ \forall n, \ \gamma_n > 0 \end{aligned} \tag{6}$$

In the formula the following notations (based on A_u) are used: $t = (x, y, z, \alpha)$, $\psi_i(t) = \psi_i(x, y, z, \alpha) = \alpha\Phi_i(x) + (1-\alpha)\Phi_i(y) - \Phi_i(z)$, where $(\Phi_i(x))$ is a family of polynomials. The line above $\overline{y} = (c^n, \psi(t))$ means $\overline{y} = 1$ if $y > 1$, $\overline{y} = (-1)$ if $y < (-1)$ and $\overline{y} = y$ if $(-1) \leq y \leq 1$ [1, 15]. The learning points are set with a pseudo random sequence. The expert relates intuitively the "learning point" (x, y, z, α) to the set A_u with probability $D_1(x, y, z, \alpha)$ or to the set B_u with probability $D_2(x, y, z, \alpha)$. The probabilities $D_1(x, y, z, \alpha)$ and $D_2(x, y, z, \alpha)$ are mathematical expectation of $f(\cdot)$ over the set of positive answers - A_u and over the set of negative answers-B_u, respectively, $D_1(x, y, z, \alpha) = M(f|x, y, z, \alpha)$, if $M(f|x, y, z, \alpha) > 0$, $D_2(x, y, z, \alpha) = (-M(f|x, y, z, \alpha))$, if $M(f|x, y, z, \alpha) < 0$. Let $D'(x, y, z, \alpha)$ is the random value:

$$D'(x, y, z, \alpha) = \begin{cases} D_1(x, y, z, \alpha) & \text{if } M(f|x, y, z, \alpha) > 0; \\ -D_2(x, y, z, \alpha) & \text{if } M(f|x, y, z, \alpha) < 0; \\ 0, & \text{if } M(f|x, y, z, \alpha) = 0. \end{cases}$$

The following decomposition is used in (6):

$$f(t^{n+1}) = \left[D'(t^{n+1}) + \xi^{n+1} \right] \tag{7}$$

In the formula above ξ denotes the uncertainty in the expert answers. We approximate $D'(x, y, z, \alpha)$ by a function of the type:

$$G(x, y, z, \alpha) = (\alpha g(x) + (1-\alpha)g(y) - g(z)), g(x) = \sum_i c_i \Phi_i(x)$$

The function $\mathbf{g(x)}$ **is an approximation of the utility** $\mathbf{u}(\cdot)$. The coefficients c_i^n take part in:

$$g^n(x) = \sum_{i=1}^{N} c_i^n \Phi_i(x), (c^n, \Psi(t)) = \alpha g^n(x) + (1-\alpha)g^n(y) - g^n(z) = G^n(x, y, z, \alpha). \tag{8}$$

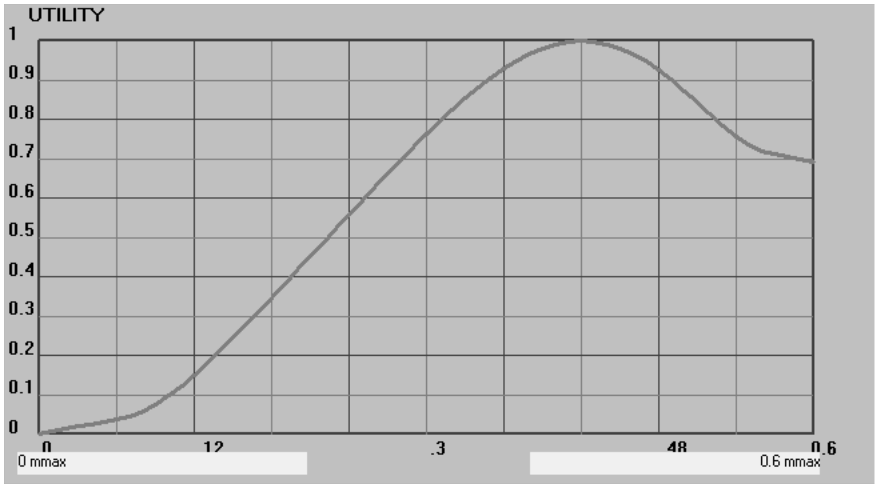

Figure 1: Utility function evaluation

The function $G^n(x, y, z, \alpha)$ is positive over A_u and negative over B_u depending on the degree of approximation of $D'(x, y, z, \alpha)$. The convergence of the procedure is analyzed in[1]. The learning points $((x, y, z, \alpha), f(x, y, z, \alpha))$ are set with a pseudo random L_{p_τ} sequence and this defines a priori the number of learning points in the procedure $(p \in \mathbf{N}, n = 2^p, 64, 128, 256, \ldots)$.

The proposed procedure and its modifications are machine learning [1, 15]. The computer is taught to have the same preferences as the DM. The DM is comparatively quick in learning to operate with the procedure. For example a session with 128 questions (learning points) takes approximately no more than 45 minutes and the utility function is evaluated with mathematical precision.

5. Growth rate evaluation of a cultivation process

The complexity of the biotechnological fermentation processes makes difficult the determination of the optimal process parameters. The incomplete information is compensated with the participation of imprecise expert estimations. Our experience is that the human estimation of the process parameters of a fermentation process contains uncertainty in the range of 10% to 25%.

Let $\mathbf{Z}$ be the set of alternatives ($\mathbf{Z} =$ specific growth rates $-\mu \equiv [0, 0.6]$) and $\mathbf{P}$ be a convex subset of discrete probability distributions over $\mathbf{Z}$. The expert "preference" relation over $\mathbf{P}$ is expressed through $(\succ)$ and this is also true for those over $\mathbf{Z}(\mathbf{Z} \subseteq \mathbf{P})$. As mentioned above the utility function is defined with precision up to affine transformation (interval scale). A decision support system for subjective utility evaluations is built and used. The results are shown on Fig.1. The utility function is approximated by a polynomial:

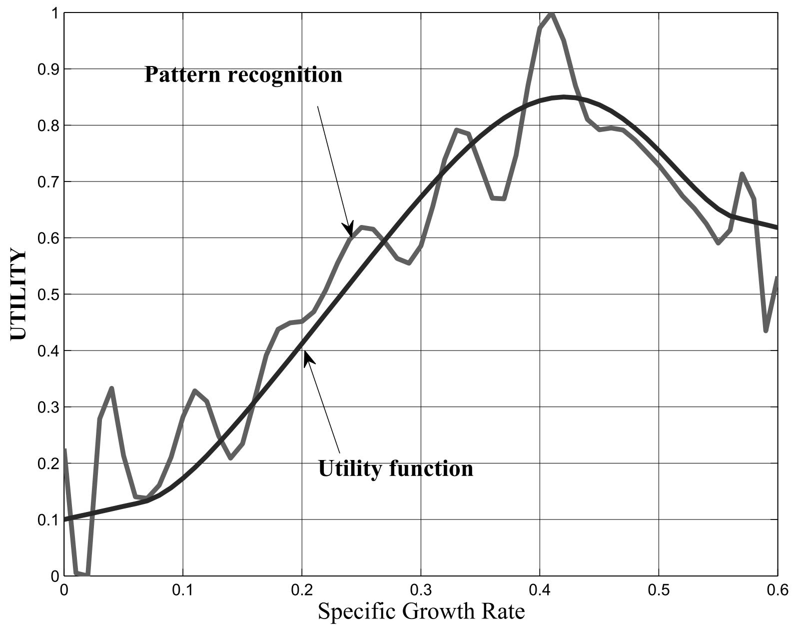

Figure 2: Pattern recognition

$$U(\mu) = \sum_{i=0}^{6} c_i \mu^i \tag{9}$$

The polynomial representation permits exact analytical determination of the derivative of the utility function and determination of the optimal technological parameters, optimal specific growth rate (optimal set point) (Fig.1) [15]. The utility is evaluated with 64 learning points. This number of questions is for a primary orientation. The seesaw line (Fig.2) is pattern recognition of A_u and B_u. This seesaw line recognizes correctly more than 97% of the expert answers. The polynomial approximation of the DM utility $u(\mu)$ is the smooth line in Fig. 2. The expert utility recognizes correctly more than 81% of the expert answers (learning points). The maximum of the utility function determines the optimal set point of the fed-batch process after the technologist. The pattern recognition is stochastic because $A_u \cap B_u = \emptyset$, since the human uncertainty appears in the mathematical presentation as additive noise.

6. Control design and stabilization in the "best" growth rate

The presentation of the control design follows the presentations in papers [15, 16, 17]. We preserve the notation $U(\cdot)$ for the DM utility. The control design is based on the solution of the following optimal control problem:

$\mathbf{Max}(U(\boldsymbol{\mu}))$, where the variable $\boldsymbol{\mu}$ is the specific growth rate, ($\boldsymbol{\mu} \in (0, \boldsymbol{\mu}_{max}]$, $D \in [0, D_{max}]$). Here $U(\mu)$ is an aggregation objective function (the utility function) and D is the control input (the dilution rate):

$$\begin{aligned}
&\max(u(\mu)), \mu \in [0, \mu_{\max}], t \in [0, T_{int}], D \in [0, D_{\max}] \\
&\dot{X} = \mu X - DX \\
&\dot{S} = -k\mu X + (S_0 - S)D \\
&\dot{\mu} = m\left(\mu_m \frac{S}{(K_S + S)} - \mu\right)
\end{aligned} \tag{10}$$

The differential equation in (10) describes a ***a continuous fermentation process*** . The Monod-Wang model permits exact linearization to Brunovsky normal form following the procedures in papers [3, 17]. The optimal solution is determined with the use of the Brunovsky normal form of model (10):

$$\begin{aligned}
\dot{Y_1} &= Y_2 \\
\dot{Y_2} &= Y_3 \\
\dot{Y_3} &= W.
\end{aligned} \tag{11}$$

In the formula above, W denotes the control input of the Brunovsky model (11). The vector (Y_1, Y_2, Y_3) is the new state vector [15]:

$$\begin{aligned}
&Y_1 = u_1 \\
&Y_2 = u_3(u_1 - ku_1^2) \\
&Y_3 = u_3^2(u_1 - 3ku_1^2 + 2k^3u_1^3) + m\left(\mu_m \frac{u_2}{(K_s + u_2)} - u_3\right)(u_1 - ku_1^2) \\
&\begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix} = \Phi(X, S, \mu) = \begin{pmatrix} \frac{X}{S_0 - S} \\ S \\ \mu \end{pmatrix}
\end{aligned} \tag{12}$$

The derivative of the function Y_3 determines the interconnection between W and D. The control design is a design based on the Brunovsky normal form and the application of the Pontrjagins maximum principle step by step for sufficiently small time periods T [2, 11, 15, 16]. The reason for the choice of such optimal control design is that the input control set in the Brunovsky form is time-dependent [9]. The interval T could be the step of discretization of the differential equation solver. The optimal control law has the analytical form [15, 16]:

$$\begin{aligned}
&D_{opt} = \ \mathbf{sign}\ \left(\left(\sum_{i=1}^{6} ic_i\mu^{(i-1)}\right)(T-t)\left[\frac{(T-t)\mu(1-2kY_1)}{2} - 1\right]\right) D_{\max} \\
&\textit{where} \\
&\mathbf{sign}\ (r) = 1,\ r > 0,\ \mathbf{sign}\ (r) = 0, r \leq 0
\end{aligned} \tag{13}$$

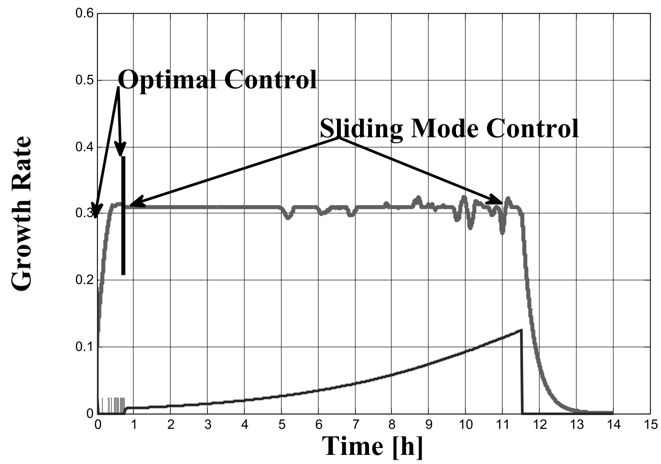

Figure 3: Stabilization of the fed-batch process

The sum is the derivative of the utility function. It is clear that the optimal "time-minimization" control is determined from the sign of the utility derivative. The control input is $D = D_{\max}$ or $D = 0$. The solution is in fact a "time-minimization" control (if the time period T_{int} is sufficiently small). The control brings the system back to the set point for minimal time in any case of specific growth rate deviations [15, 16]. The control law of the fed-batch process has the same form because $D(t)$ is replaced with $F(t)/V(t)$ in Monod-Wang model (5). Thus, the feeding rate $F(t)$ takes $F(t) = F_{\max}$ or $F(t) = 0$, depending on $D(t)$ which takes $D = D_{\max}$ or $D = 0$.

We conclude that the control law (13) *brings the system to the set point (optimal growth rate) with a "time minimization" control, starting from any deviation of the specific growth rate. We use this control law as a main part in a more complex chattering control law solution for stabilization of the system in the "best" growth rate position* [6, 15, 16].

This type of control may be used only for cumulative criteria for which the Bellman principle is valid in the optimal control [9]. For example, such are the amount of biomass at the end of the process and the time-minimization optimal control.

The deviation of the fed-batch process with this chattering control is shown on Fig.3. After the stabilization of the system in equivalent sliding mode control position the system can be maintained around the optimal parameters with sliding mode control (Fig.3) [6, 15, 16]. The iterative utility function design and the iterative corrections in the DM preferences permit adjustment of the control law and of the optimal control final results in agreement with the changes in the opinion of biotechnologist. The procedure could be interprets as learning procedure in the two opposite directions, in direction to biotechnologist or in

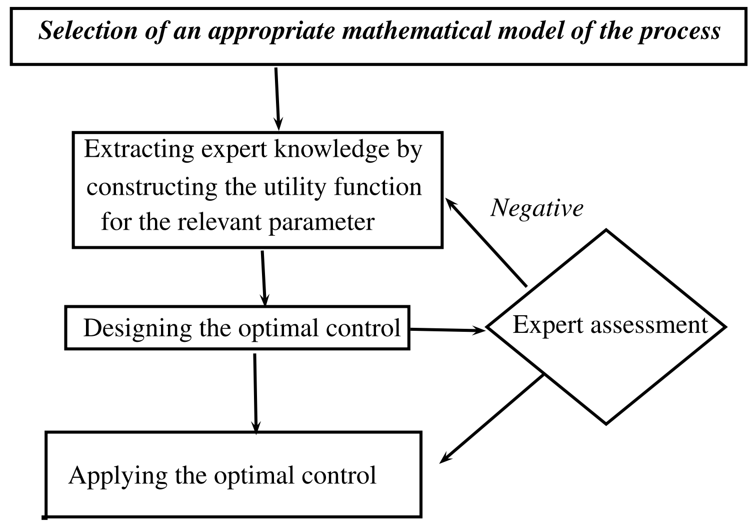

Figure 4: The methodology for extracting experts knowledge for the design of the control law

direction to the final optimal solution.

7. Final remarks

Here we would like to present a flow-chart of the methodology used to once more emphasize the generality of such approach which can be used succesffuly in other areas. The flowchart on Fig. 4 will serve as a basis for a detailed generalized net ([21]) model of the methodology to be developed in future work. Here we present only the main steps, as the technical details are specific for each process and implementation. For instance, the degree of the polynomial used to approximate the utility function may vary. What is important to note is that the human preferences are quantified by the construction of the utility function and at the same time the expert may further input new preferences based on the observed result, so with each iteration both the quantified evaluations and the qualitative reasoning of the expert are improved.

8. Conclusions

In the paper a mathematical utility evaluation procedure for elimination of the uncertainty in the decision-makers preferences and evaluation of the "best" technological conditions is proposed. The approach permits iterative and precise evaluation of the "best" specific growth rate of the fed-batch process and iterative control design in agreement with the DMs preferences as maximum of this utility function.

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