

# Adlers Ingenjörsdata

Bertil Persson Avdelning TM OKG AB 572 83 Oskarshamn

Hej!

Översänder rapporten "State Estimation Based on Mathematical Modelling and Plant Measurement" samt härtill rörande MATHCAD-filer på diskett.

Vi hoppas att rapporten motsvarar Era förväntningar och vi tackar Er för ett mycket gott samarbete.

Med vänlig hälsning

Denes Szentivanvi

Faktura samt F-skattesedel bifogas.

		ISTREHA	AT DOKUMENT
Administrativ	Reg nr 96-00290		
Arendenr 2	96	0105	Mattagare /Bet
Dokumentnamn	Ra	pport	3.0
Distribution	er,	BNIV	
		*************	

# STATE ESTIMATION BASED ON MATHEMATICAL MODELLING AND PLANT MEASUREMENT

Dr. Béla Paláncz

Dénes Szentiványi

Adlers Ingenjörsdata

Sollentuna 951215

# **CONTENT**

ABSTRACT	3
INTRODUCTION	б
1. MEASUREMENT CORRECTION	7
1.1 Linearization of the balance equation	
1.2 Computing corrections	9
1.3 Condition for accepting measurements	10
1.4 Detecting outliers	11
2. PARAMETER ESTIMATION	13
2.1 Linearization of the model	13
2.2 Parameter estimation without constrains	
2.3 Application ridge-regression	14
2.4 Parameter estimation with constrains	14
2.5 Computing upper and lower bound for the estimated values	15
3. SUMMARY	16
LITERATURE	17
APPENDIX	18

# **ABSTRACT**

#### Aim of the study

The aim of this study is to develop a methodology for parameter estimation (PE) of the main processunits of a nuclear power plant. These parameters can be, the measure of fouling of heat exchangers (pre- and reheaters), efficiency of water separators, thermodynamic efficiency and Stodola-number of steam turbines etc. The employed method must be based on field measurement of the state variables, namely, temperatures, pressures, flow rates etc., as well as on a mathematical model of the process. This model is represented by a flow-sheeting algorithm coded in the PROBERA flow sheeting computer program.

#### Design of the parameter estimation

First of all the PE procedure must be designed. Parameters, which represent the state of the units, have to be selected. Then measurement points and state variables, which can be reliably measured as well as computed from the process model, must be chosen. In addition these selected state variables should have as strong correlation as possible with the selected parameters. Generally, the number of the parameters is limited because of the stability of the applied numerical method, so their numbers are mostly less than 20. The number of the considered state variables must be more than that of the parameters, to ensure over-determined system, consequently reliable estimation.

# PE procedure

The PE procedure can be carried out in three steps

- analysis of the measurements (pre-processing phase)
- determination of new parameter values (processing phase)
- analysis of the result from engineer point of view (post-processing phase)

For PE procedure one can use linearized model, because normally change of parameters is taking place slowly, so apart from some abnormal situations, the new parameter values will be not very far from the old ones. It is also useful to employ normalised variables with the computed values as references.

#### Pre-processing phase of PE

In this phase, first one has to decide whether parameter estimation is possible at all.

If the measurement error, which consists of measuring error caused by process noise or systematical measuring error, error of the measuring device calibration error, zero-point error etc., and the error of the transducers, is higher than the modelling error, namely the difference between the measured and the computed value, then further analysis is not rational.

If the modelling error is higher than the measurement error, then "wrong" measurements, so called outliers have to be filtered out by measurement correction, if there is any. It means that measured values will be corrected in such a way, that they will satisfy the balance equations of the flow-sheet model and at the same time they represent the minimal deviation from the original measured values. On the bases

of the residual of this minimisation problem,  $\chi^2$  test can be carried out, to check, whether the measurement values are acceptable or not. If they are acceptable, then no more investigation is necessary, but in opposite case we can look for outliers. A statistical index  $\gamma$  can be computed for every measured variable. If this  $\gamma$  index is close to one in absolute value, then this measured value can be

qualified as outlier. It means, that this measurement can be repeated, left out or substituted by its computed value. PE process is carried out, even if the  $\chi^2$  test remains negative after the elimination of outliers.

#### Processing phase of PE

As first step, standard linear parameter estimation using least square method is employed. If some new, estimated parameter value fall into a too wide range, with other words their new values differ from the original ones too much, then the so called ridge-parameter estimation can be employed to make the PE procedure more robust.

If we want to use constrains for certain parameters, i.e. their change can be only positive, then constrained linear or alternatively unconstrained non-linear parameter estimation are suggested.

#### Post-processing phase of PE

After the determination of the new values of the parameters, different statistics can be computed to characterise the quality of the PE procedure. It is also possible to compute the upper and lower bound of the parameter values at a certain confidence level.

Analysing these characteristics and taking into consideration engineering point of views, one may go back to phase processing, and can use an other estimation algorithm, or even may go back to phase preprocessing, and select new measured variables or parameters in order to make the result of PE more realistic.

# Illustration of PE procedure

In order to illustrate this methodology described above, PE was carried out for the PROBERA O2\_322 circuit, at three different timepoints. In that case three inputs, eleven outputs and five parameters were selected. We could detect "wrong" measurements and our result had good agreement with result provided by the parameter estimation module of PROBERA.

The circuit PROBERA OSCAR3 was also investigated in two different versions. First, two inputs and 29 outputs as well as 16 parameters (fouling of the different type of heaters) were considered. Here, we also could find outliers, and the PE procedure worked successfully. In the second version we selected more realistic and more important characteristics of the circuit units as parameters, namely thermodynamical efficiency of turbine stages, efficiency of water separator, fouling of heaters etc. According to the result of these investigations the application of this PE seems to be very promising.

In the Appendix one can find the MATHCAD programs of these five illustrative examples.

#### Tasks for the future

In order to add this PE procedure to the PROBERA flow-sheeting program the following tasks must be carried out:

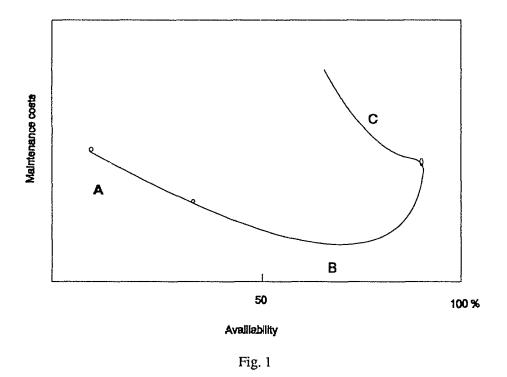
- 1. Measurement points must be selected as many as possible.
- 2. The sources of measurement error must be detected and estimated, namely, system noise, calibration error, zero point error, systematical measuring error and the error of the transducers. It would be also useful to analyse the model computing reactor thermal power, as input information.

- 3. Parameters must be selected. Here, in order to minimise the chance of misleading estimation, so called multilevel, or nested estimation could be considered. For example, first only the overall heat transfer coefficient can be estimated, and then the value of the heat conduction resistance and internal and external heat transfer coefficients can be considered as parameters at the second level.
- 4. These three steps could be summarised in one menu point called as Design Phase. The user can select variables and parameters freely, and check their compatibility.
- 5. Pre-processing algorithm can be coded as second menu point containing the steps of this PE phase.
- 6. The third menu point as processing phase must contain different estimation procedures and a simple knowledge base could support the user to select the most appropriate method. Linear estimation with least square objective, ridge estimation, linear estimation with constrained and non-linear estimation with constrained would be the most probable candidates, however other methods having other type of objectives (i.e. maximum likelihood) could also be considered.
- 7. Post-processing phase concerns different statistics, as residual, weighted empirical standard deviation, Durbin-Watson D statistics, the covariance matrix, the confidence interval etc., there should also be a built-in knowledge base that could help the user to understand the physical meaning of the result and to accept it or reject it and carry out a new estimation.

  This PE procedure could be a module in PROBERA flow-sheeting program and could improve its ability for state estimation of power plant units significantly.

# INTRODUCTION

Reliability and efficiency are among the most important features of up-to-date operation of plants where technological processes of industrial chemistry and energy production are taking place. Of course, reliability and efficiency are closely interrelated as a reduction in the efficiency of major equipment, losses in production due to unforeseen breakdown and increased costs of repair affect the economic efficiency equally unfavourably. Figure 1 shows the theoretical relationship between maintenance costs and availability. In this Figure, preventive maintenance is minimum along section 'A' and thus availability in terms of percentage of actual hours of operation as compared with the planned hours reduces due to frequently occurring breakdowns, accompanied with increasing costs resulting from subsequent repairs. The correct preventive maintenance schedule along section 'B' results in increasing availability with also the costs of preventive and subsequent maintenance lying well below the costs according to strategy 'A'. At the same time, an over-estimated preventive maintenance demand like in strategy 'C' results in increasing standstill that is in reducing availability /1/. Hence, in fact, the relationship between availability and maintenance costs can be optimised although in practice it is difficult to express this optimum numerically.



The close correlation between reliability and efficiency of operation comes in focus especially if reliability implies not only unforeseen standstill prevention but also control of disorders in major equipment which, although not preventing the equipment from operating at given instant, may reduce the efficiency of operation considerably and result sooner or later in a temporary and partial reduction in performance due to inevitable repair /2/.

Measurements alone are not enough to determine reduction in the efficiency of power plant operation. Use of a mathematical model describing given process, usually together with material and energy balances, is therefore necessary /3,4/.

The energetic efficiency of certain equipment like turbines and heat exchangers may reduce during operation as a result of leakage, contamination etc. These changes are typically slow and they have no direct drastic effect upon operation.

A mathematical model describing the process is used on the basis of measurement of certain typical operating variables to investigate the state that is to answer the question whether the difference between the measured values and those supplied by the model resulted from erroneous measurements or the state of some major equipment changed so that the model parameters characteristic of that equipment were no longer valid. What we want to know is what kind of change has occurred or is about to develop in which of the equipment.

# 1. MEASUREMENT CORRECTION

The model parameters characteristic of the energetic state of the equipment like stage efficiency or thermal transmission factor etc. are based essentially on parameter estimation. However, measurement correction is necessary to decide whether new parameters have to be determined that is parameter estimation has to be carried out, or the significant difference between the calculated and measured values resulted from erroneous, failing measurements only /5/.

Values measured in the course of operation include pressure, differential pressure, temperature etc. For different reasons (instability in time, error of measuring device, recurrent measuring error etc.), the values so obtained are more or less erroneous. A condition for acceptability of the measurements is that they satisfy the material and energy balances describing the process.

#### 1.1 Linearization of the balance equation

The process is usually described by the following non-linear input-output model:

$$y = F(p, x). (1.1)$$

where y and x are the vector of the output and input variables, respectively and p is the vector of the parameters.

Linearizing around the state of operation according to input variables we get:

$$\mathbf{y} = \mathbf{F}(\mathbf{p}_{old}, \mathbf{x}_{m}) + \left[\frac{\partial \mathbf{F}_{i}}{\partial \mathbf{x}_{j}}\right]_{\mathbf{p}_{old}, \mathbf{x}_{m}} (\mathbf{x} - \mathbf{x}_{m}).$$
or
$$\mathbf{y} = \mathbf{y}_{\epsilon} + \mathbf{A}(\mathbf{x} - \mathbf{x}_{m}).$$
(1.2)

where -  $\mathbf{p}_{old}$ , the original parameters, before the parameter estimation

- x<sub>m</sub>, the vector of the measured values
- $\mathbf{y}_{c}$ , the computed values

Essentially, equalisation is a correction of the values less deviating from the measured values in a certain sense and at the same time satisfying the heat and material balances constituting the heat-flow diagram model. It is usually minimisation in a weighted quadratic sense where the weight matrix is a reciprocal of the diagonal matrix set up of mean square deviation of measurements.

New variables are introduced for the linearized model in order to use the usual form:

$$Y = \begin{bmatrix} x \\ y \end{bmatrix}$$
 and  $b = y_c - Ax_m$  (1.3)

Thus the original linear model can be written in the following form:

$$\mathbf{WY} - \mathbf{b} = \mathbf{0} \tag{1.4}$$

where

$$\mathbf{W} = \begin{bmatrix} -\mathbf{A} : & +\mathbf{E} \end{bmatrix} \tag{1.5}$$

Let

$$\mathbf{Y}_{m} = \begin{bmatrix} \mathbf{X}_{m} \\ \mathbf{y}_{m} \end{bmatrix} \tag{1.6}$$

be the vector of measurement results. Now quadratic form

$$Q(Y) = (Y - Y_{m})^{T} V^{-1} (Y - Y_{m})$$
 (1.7)

is minimised by linear balance equalisation, where the weight matrix is a diagonal matrix containing the square of the standard deviation of the measured input and output variables:

$$\mathbf{V} = \begin{bmatrix} \sigma_{\mathbf{x}_{m1}}^2 & & & \\ & \sigma_{\mathbf{x}_{m2}}^2 & & \\ & & \cdot & \\ & & \cdot & \\ & & & \sigma_{\mathbf{y}_{mn}}^2 \end{bmatrix}$$
(1.8)

Now our task is to find Y which minimises Eq.(1.7) and at the same time satisfies Eq.(1.4). It means to find Y which satisfies the balance equations and is so close to the measured values,  $Y_m$  as possible.

# 1.2 Computing corrections

Let us introduce the correction vector, or the error of measurement as

$$c = Y - Y_{m} \tag{1.9}$$

and the balance-error vector is:

$$\mathbf{f} = \mathbf{W}\mathbf{Y}_{_{\mathbf{n}\mathbf{i}}} - \mathbf{b} \tag{1.10}$$

Then our task to minimise

$$Q(\mathbf{c}) = \mathbf{c}^{\mathrm{T}} \mathbf{V}^{-1} \mathbf{c} \tag{1.11}$$

under the condition

$$\mathbf{Wc} + \mathbf{f} = \mathbf{0} \tag{1.12}$$

A problem (1.11-1.12) can be solve using Lagrange multiplicator method. The new objective function is

$$L(\mathbf{c}, \lambda) = \mathbf{c}^{\mathrm{T}} \mathbf{V}^{-1} \mathbf{c} + \lambda^{\mathrm{T}} (\mathbf{W} \mathbf{c} + \mathbf{f})$$
 (1.13)

The extremum must satisfy the following necessary conditions

$$\frac{\partial \mathbf{L}}{\partial \mathbf{c}} = 2\mathbf{V}^{-1}\mathbf{c} + \mathbf{W}^{\mathrm{T}}\boldsymbol{\lambda} = \mathbf{0}$$
 (1.14)

$$\frac{\partial \mathbf{L}}{\partial \lambda} = \mathbf{W}\mathbf{c} + \mathbf{f} = \mathbf{0} \tag{1.15}$$

From (1.14) we get

$$\mathbf{c} = -\frac{1}{2} \mathbf{V} \mathbf{W}^{\mathrm{T}} \lambda \tag{1.16}$$

and substituting this into (1.15) and expressing  $\lambda$ 

$$\lambda = 2(\mathbf{W}\mathbf{V}\mathbf{W}^{\mathrm{T}})^{-1}\mathbf{f} \tag{1.17}$$

Then from (1.14) the optimal correction is

$$\hat{\mathbf{c}} = -\mathbf{V}\mathbf{W}^{\mathrm{T}} (\mathbf{W}\mathbf{V}\mathbf{W}^{\mathrm{T}})^{-1} \mathbf{f}$$
 (1.18)

The corrected measured values are

$$\mathbf{Y}_{n} = \mathbf{Y}_{n} + \hat{\mathbf{c}} \tag{1.19}$$

# 1.3 Condition for accepting measurements

Now we have to check, whether these measurements,  $\mathbf{Y}_{m}$  can be accepted or not. Substituting  $\hat{\mathbf{c}}$  into (1.11) we get the measure of error

$$q^2 = Q(\hat{\mathbf{c}}) = \mathbf{f}^T (\mathbf{W} \mathbf{V} \mathbf{W}^T)^{-1} \mathbf{f}$$

This measure is *invariant* to the scaling of the balance equations. It means that it depends neither on the measurement units of Y nor the way of the derivation of the balance equations.

According to (1.12), there is a homogen, linear relation between the error of measurement c and the balance error f. Of course, because w is not quadratic, there are more variables than balance equations. The freedom of the system is the difference of the number of columns and of rows.

If we suppose that the c error has normal distribution with 0 mean, then f also has normal distribution with 0 mean. Using linear transformation it is possible to transform f into  $\varphi$  which has zero mean with unit deviation.

$$\varphi = (\mathbf{W}\mathbf{V}\mathbf{W}^{\mathrm{T}})^{-\frac{1}{2}}\mathbf{f} \tag{1.20}$$

Therefore  $\boldsymbol{\phi}$  has similar distribution as  $\boldsymbol{f}$  . Because

$$q^2 = \varphi^T \varphi \tag{1.21}$$

Consequently q has also normal distribution with 0 mean and with unit deviation , therefore  $q^2$  has  $\chi^2$  central distribution with the freedom of the system. In our case this is equal NI, the number of the input variables x, because for every output variable we have one balance equation, namely W has NI + NO columns and NO rows, where NO is the number of the output variables of the linearized model (1.2). We shall use this information to decide, whether the measurement can be accepted or not. We have to check whether the measurement errors  $\hat{c}$  satisfies the hypothesis namely normal distribution with 0 mean. Now we shall test the consequence of our hypothesis namely  $q^2$  has  $\chi^2$  distribution with NI freedom. Our hypothesis can be accepted if

$$q^2 \le \chi^2_{NI,p} \tag{1.22}$$

where  $\chi_{NI,p}$  is the value of the  $\chi^2$  (khi) distribution with freedom NI and at confidence level p. Usually, p=0.95 is used.

If the relation (1.22) is not true, we discard the hypothesis and suppose that the measurements have exceptional error.

# 1.4 Detecting outliers

If exceptional error has been detected, (1.22) was not true, then let us suppose that for one of the measured variables which has index r, the *mean* of measurement error not zero.

$$E(c_{\cdot}) = h \neq 0 \tag{1.23}$$

or

$$E(\mathbf{c}) = \mathbf{e} \cdot \mathbf{h} \tag{1.24}$$

where  $c_r$  is the r-th component in vector  $c_r$  and  $e_r$  the unit vector shows in the direction of the r-th coordinate axis.

Applying transformation (1.20)

$$\mathbf{M} = (\mathbf{W}\mathbf{V}\mathbf{W}^{\mathsf{T}})^{\frac{1}{2}}\mathbf{W} \tag{1.25}$$

Equation (1.12) can be written as

$$\mathbf{Mc} + \mathbf{\varphi} = 0 \tag{1.26}$$

Then taking the mean value of (1.26), the mean of  $\varphi$  or  $-\varphi$  (the sign is not interesting)

$$E(-\phi) = E(Mc) = ME(c) = Me_h = m_h$$
 (1.27)

It means that  $\phi$  must be parallel to  $m_r$ 

$$\mathbf{m}_{\cdot} = \mathbf{M}\mathbf{e}_{\cdot} \tag{1.28}$$

which is r-th column vector in M matrix.

Therefore for the exceptional error  $\mathbf{c}_r$ , the so called Almásy gamma vector /5/ is:

$$\gamma_r = \cos(\mathbf{m}_r \mathbf{\phi}) = 0 \tag{1.29}$$

So we have to compute the angle between every column vector of  $\,M\,$  and  $\,\phi$  , and if this Almásy  $\,\gamma_{\,\tau}\approx 1\,$  then this r-th measurement is suspected to have exceptional error.

Because in case of vectors a and b

$$\cos(\mathbf{a}, \mathbf{b}) = \frac{\mathbf{a}^{\mathsf{T}} \mathbf{b}}{(\mathbf{a}^{\mathsf{T}} \mathbf{a})^{\frac{1}{2}} (\mathbf{b}^{\mathsf{T}} \mathbf{b})^{\frac{1}{2}}}$$
(1.30)

then

$$\gamma_{j} = \frac{\mathbf{m}_{j}^{T} \boldsymbol{\varphi}}{(\mathbf{m}_{j}^{T} \mathbf{m}_{j})^{\frac{1}{2}} (\boldsymbol{\varphi}^{T} \boldsymbol{\varphi})^{\frac{1}{2}}} \qquad j = 1, 2, \dots, NI + NO$$
(1.31)

$$\gamma = \frac{1}{q} \left[ \operatorname{diag}(\mathbf{h}) \mathbf{W}^{\mathrm{T}} (\mathbf{W} \mathbf{V} \mathbf{W}^{\mathrm{T}})^{-1} \mathbf{f} \right]$$
 (1.32)

Considering the transformation the vector of Almásy y can be computed as

$$\mathbf{H} = \mathbf{W}^{\mathrm{T}} (\mathbf{W} \mathbf{V} \mathbf{W}^{\mathrm{T}})^{-1} \mathbf{W}$$
 (1.33)

$$\mathbf{h}_{j} = (\mathbf{H}_{j,j})^{\frac{1}{2}}$$
  $j = 1, 2, ..., NO + NI$  (1.34)

and

$$\operatorname{diag}(\mathbf{h}) = \begin{bmatrix} \mathbf{h}_1 \\ \mathbf{h}_2 \\ & & \\ & & \\ & & \\ & & \mathbf{h}_{NO+NI} \end{bmatrix}$$
 (1.35)

where

NI - the number of input variables NO - the number of output variables

# 2. PARAMETER ESTIMATION

In case the  $\chi^2$  test is negative, (1.22) is not true we have to check whether one of the variables has Almásy's gamma near to one. If it is so then this variable can be deleted or its measured value can be substituted with the computed value or the measure can be repeated. If we do not find such a variables then parameter estimation will be carried out.

Hence, if the  $\chi^2$  test is negative but a value near 1 of Almásy's gamma is not obtained for any of the measured variables, it can be rightly assumed that a change has taken place in the state of equipment, resulting in a new state that can not be represented by the value of model parameter associated with the old state. E.g. also model parameter kF characteristic of the value of the heat transfer ability for given heat exchanger shall be reduced accordingly for the sake of appropriate modelling in case of contaminated heat transfer surfaces.

#### 2.1 Linearization of the model

Since the changes are slow and thus difficult to detect them, a linearized model is used again where linearization according to the model parameters is also carried out. That is

$$y = y_c + A(x - x_m) + B(p - p_{old})$$
 (2.1)

where B is the Jacobi matrix.

$$\mathbf{B}_{i,j} = \left(\frac{\partial \mathbf{F}_i}{\partial \mathbf{p}_j}\right)_{\mathbf{p},j} \tag{2.2}$$

and  $\mathbf{x}_{m}$  is the vector of the measured input variables,  $\mathbf{p}_{old}$  is that of the old parameters.

#### 2.2 Parameter estimation without constrains

Taking into consideration this identity

$$\mathbf{x} = \mathbf{x}_{m} + \mathbf{E}(\mathbf{x} - \mathbf{x}_{m}) \tag{2.3}$$

and introducing variables

$$\mathbf{Y}_{p} = \begin{bmatrix} \Delta \mathbf{x} \\ \Delta \mathbf{y} \end{bmatrix}$$
  $\mathbf{X}_{p} = \begin{bmatrix} \Delta \mathbf{x} \\ \Delta \mathbf{p} \end{bmatrix}$  and  $\mathbf{M} = \begin{bmatrix} \mathbf{E} & \mathbf{0} \\ \mathbf{A} & \mathbf{B} \end{bmatrix}$  (2.4)

where

$$\Delta x = x - x_{m}$$

$$\Delta y = y - y_{c}$$

$$\Delta p = p - p_{old}$$
(2.5)

the linear model (2.1) can be expressed as

$$Y_{p} = MX_{p} \tag{2.6}$$

As the layout of the variables shows (2.4), now not only the parameter vector **p** but also the input vector is present on the right-hand side that is also the input vector shall be determined in the course of the estimation process.

With matrix V used again as a weight matrix, the expression to be minimised will be

$$J(X_{p}) = (Y_{p} - MX_{p})V^{-1}(Y_{p} - MX_{p})$$
 (2.7)

The solution can be written in similar way then in case the measurement correction, namely

$$\hat{\mathbf{X}}_{p} = (\mathbf{M}^{T} \mathbf{V}^{-1} \mathbf{M})^{-1} \mathbf{M}^{T} \mathbf{V}^{-1} \mathbf{Y}_{p}$$
 (2.8)

# 2.3 Application ridge-regression

Sometimes it can happen that one of or more of eigenvalues of the matrix  $\mathbf{M}^T \mathbf{V}^{-1} \mathbf{M}$  is/are very small, because of the weak correlation between the measured variables and parameters. In that case we can use the ridge-regression, which is a distorted estimation /6/. The optimal estimation is

$$\hat{\mathbf{X}}_{p} = (\mathbf{M}^{T} \mathbf{V}^{-1} \mathbf{M} + \lambda \mathbf{E})^{-1} \mathbf{M}^{T} \mathbf{V}^{-1} \mathbf{Y}_{p}$$
(2.9)

This  $\lambda$  so cold ridge parameter increases the small eigenvalues of  $M^TV^{-1}M$ . The estimation of a parameter  $X_{p_i}$  is said to be stable if it is invariant to the change of  $\lambda$ .

Employing this method one can select and filter out parameters which can be "badly" estimated, and their reliable estimation may need new output variables to be considered and measured.

# 2.4 Parameter estimation with constrains

Note that in practice, an arbitrary domain one may use for minimisation of (2.8) is usually not permissible. Namely, an unconstrained linear parameter estimation can yield also a solution resulting in minimum value for J with, however, the physically optimum values of  $X_p$  falling within the inadmissible domain (e.g. the active heat transfer coefficient increases).

This means that for certain parameters

$$\mathbf{X}_{\mathbf{p}_i} \ge 0 \tag{2.10}$$

constrain must be considered.

Instead of minimising (2.7) under the condition (2.10), we can transform the linear objective function (2.7) with its constrain (2.10) into a non-linear objective function without constrain.

Let us introduce for this the variables

$$\alpha_i^2 = X_{p_i} \tag{2.11}$$

Then for every value of  $\alpha_i$ ,  $X_{p_i}$  is not negative if the solution is real. The objective function (2.7) can be written in the following form:

$$\mathbf{J}(\mathbf{X}_{p_1}, \mathbf{X}_{p_2} ... \alpha_i^2) = \sum_{j=1}^{NI+NO} \frac{\left[\mathbf{Y}_{p_j} - \left(\mathbf{M}_{j,1} \mathbf{X}_{p_1} + \mathbf{M}_{j,2} \mathbf{X}_{p_2} + .... + \mathbf{M}_{j,i} \alpha_i^2 + ....\right)\right]^2}{\mathbf{V}_{i,j}}$$
(2.12)

where

NI - number of input variables and NO - number of output variables.

Now, we can minimise  $J(X_{p_1}, X_{p_2}, ..., \alpha_i^2, ...)$  without constrains, then using (2.11) to get  $X_{p_i}$ .

# 2.5 Computing upper and lower bound for the estimated values.

In order to estimate the "fitting" of the parameters, we can compute their upper and lower limit at a certain confidence level assuming that the probability distribution of the measurement error has normal distribution.

The residual deviation is the value of (2.7) at  $\mathbf{X}_p = \hat{\mathbf{X}}_{p,0}$ . Then the residual deviation can be determined as

$$s_r^2 = \frac{J(\hat{X}_p)}{f} \tag{2.13}$$

where f is the number of freedom.

$$f=NI+NO-(NI+NP)=NO-NP$$
 (2.14)

Now the covariance - matrix of the estimation, can be estimated in the following way

$$c = s_r^2 (M^T V^{-1} M)^{-1}$$
 (2.15)

Then the main diagonal elements of this matrix are square of the deviation of the parameters. Assuming normal distribution, the interval of upper and lower bound of the parameters is

$$\hat{\mathbf{X}}_{p_i} - \sqrt{\mathbf{c}_{ii}} \mathbf{t}_{f,z} \le \mathbf{X}_{p_i} \le \hat{\mathbf{X}}_{p_i} + \sqrt{\mathbf{c}_{ii}} \mathbf{t}_{f,z}$$
 (2.16)

where  $t_{f,z}$  the value of the Student distribution with f freedom at  $\epsilon$  % confidence level and

$$z = 1 - \varepsilon/100 \tag{2.17}$$

#### 3. SUMMARY

Now, we can summarise the recommended algorithm of the state estimation procedure.

Using measured input values, the measured output variables can be computed and the computed and measured values can be compared. The deviation between these two type of values is called the "model"-error, caused by wrong measurement or modelling error, or incorrect, not updated model parameters.

One can utilise the measurement from the point of view of estimation of new state, if the measurement error of the measurement devices are smaller than the "model"-error. If it is true we have to check whether measurements are fitting "close enough" to the model or not, and outliers must be filtered out (see measurement corrections, outlier detection).

If there are outliers then their measured values can be substituted with the computed values or they can be left out. If even after this filtration the fitting is not "close enough" - assuming that the modelling error is negligible - new model parameter can be estimated. We have to analyse whether the measured variables are adequate for estimating the considered parameters. This means that one has to study matrix B, (2.2) which shows the relations between measured variables and parameters, as well as one can employ ridge-regression and other statistical test (Durbin-Watson D statistics or Kolmogrov test) to determine the goodness of the estimation.

# LITERATURE

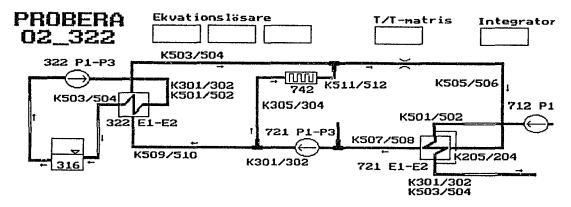
- 1. Davis, D. A. et. al.(1986): Availability of Thermal Generating Plant, Proceedings of the 13rd World Energy Conference, Working Group 1, Cannes, France, pp. 287-295
- 2.Chiv, C., (1986): Identify Electric Output Losses of PWR Nuclear Plants, Power, Sept. pp. 35-39
- 3. Gilles, E. D. Niaklaus, E. Palke, M., (1986): Sensortechnik in der Chemie Status und Trend, Chem. Ing. Techn. 58., pp. 557-564
- 4. Paláncz, B., (1988): A Modular Approach to the Simulation of Steam Turbine Cycles, Applied Energy 30., pp. 147-152
- 5. Almásy, G. A., Sztano, T., (1975): Checking and Correction of Measurements on the Basis of Linear System Model, Problems of Control and Information Theory 4. pp. 57-69
- 6. Hoerl, A. E. Kennard, R. W., (1970): Ridge regression: Biased estimation for non-orthogonal problems, Technometrics, 12, pp. 55-57

# **APPENDIX**

# **Parameter Estimation**

This MCAD program illustrates the parameter estimation procedure described in our report.

#### Flow-sheet of PROBERA 02\_322



The measured input and output variables as well as parameters were selected as below:

These values were measured.

Parameters:

p1 - Flow resistance of cold stream in 322 (-)  
p2 - Flow resistance of warm stream in 712 (-)  
p3 - Flow resistance in 721 (-)  
p4 - Fouling in primer side of heater 322 (m)  
p5 - Fouling in primer side of heater 721 (m)
$$p := \begin{cases} 159.42 \\ 38.29 \\ 81.577 \\ 2.1 \cdot 10^{-5} \end{cases}$$

These parameter values were the original, standard values in the PROBERA flow-sheeting program.

Computed values of the Output using nonlinear Model represented by PROBERA:

#### **Measurements Errors:**

The measurement error for temperature measurements was 0.1 °C, except x1, for it was 0.5 %. For flow rates 1.5 % and 2 % relative errors were considered, respectively.

for Input: 
$$\sigma_{x} := \begin{bmatrix} x_{m_{0}} \cdot 0.005 \\ x_{m_{1}} \cdot 0.02 \\ 0.1 \end{bmatrix} \qquad \qquad \sigma_{y} := \begin{bmatrix} y_{c_{0}} \cdot 0.015 \\ 0.1 \\ 0.1 \\ y_{c_{3}} \cdot 0.015 \\ 0.1 \\ 0.$$

In order to decide whether parameter estimation is necessary or not, the commulative measurement and modelling errors are computed. The modeling error is the sum of the differences between measured and the corresponding computed values.

#### Inspection

Comparing Measurement Error with Modelling Error:

Modeling Error:

Number of Output: NO := 11 
$$i := 0...NO - 1$$
  $MoE_i := |y_{m_i} - y_{c_i}|$ 

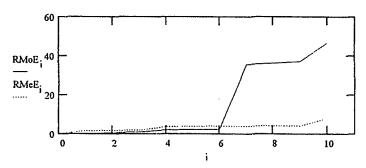
Commulative Modelling Error:

$$RMoE_0 := 0 \quad RMoE_{i+1} := RMoE_i + MoE_i$$

Commulative Measurement Error:

$$RMeE_0 := 0$$

$$RMeE_{i+1} := RMeE_i + \sigma_{y_i}$$



Comparing modelling error and measurement error

This figure indicates, that the flow sheeting modell is not adequate, or there are wrong measurements or certain changes took place in the state of process units, because the model-parameters are not adequate. We suppose that the flow-sheeting modell is verified, so only the possibility of the two other cases will be considered

For further computation, the variables can be normalized using the computed values as references

Normalized vectors:

$$NI := 3 \qquad \qquad i := 0 ... \, NI - 1 \qquad \qquad Nx_{m_i} := 1 \qquad \qquad N\sigma_{x_i} := \left(\frac{\sigma_{x_i}}{x_{m_i}}\right)$$

$$i := 0.. \text{ NO} - 1$$
  $\text{Ny}_{m_i} := \frac{y_{m_i}}{y_{c_i}}$   $\text{No}_{y_i} := \frac{\sigma_{y_i}}{y_{c_i}}$   $\text{Ny}_{c_i} := 1$ 

First, we shall looking for wrong measurements, so called outliers.

#### **Measurement Correction**

Model linearization using numerically computed Jacobi matrix:

To create the Jacobian matrix for measurement correction, the output variables are computed in two different points of the input variables represented by the first and third elements of vectors Tihe second value is the measured value of the input variable.

$$\mathbf{x1} := \begin{pmatrix} 23.52 \\ 23.76 \\ 24 \end{pmatrix} \qquad \mathbf{x2} := \begin{pmatrix} 0.31 \\ 0.32 \\ 0.33 \end{pmatrix} \qquad \mathbf{x3} := \begin{pmatrix} 17.184 \\ 17.358 \\ 17.532 \end{pmatrix}$$

We normalize these input values, too.

$$i := 0..NI - 1$$

$$Nx1_{i} := \frac{x1_{i}}{x_{m_{0}}}$$
  $Nx2_{i} := \frac{x2_{i}}{x_{m_{1}}}$   $Nx3_{i} := \frac{x3_{i}}{x_{m_{2}}}$ 

# Computing function values, Yikf at x1, x2, x3,

#### Normalization again.

$$i := 0.. NO - 1$$

$$NY122_{i} := \frac{Y122_{i}}{y_{c_{i}}} \qquad NY322_{i} := \frac{Y322_{i}}{y_{c_{i}}} \qquad NY212_{i} := \frac{Y212_{i}}{y_{c_{i}}}$$

$$\begin{bmatrix} 100.07 \\ 23.847 \\ 18.738 \\ 124.89 \\ 18.065 \\ Y232 := \begin{bmatrix} 100.07 \\ 23.845 \\ 18.489 \\ 17.907 \\ 22.134 \\ 54.345 \\ 22.405 \\ 18.003 \\ 18.003 \\ 18.998 \end{bmatrix}$$

$$\begin{bmatrix} 100.07 \\ 23.845 \\ 18.601 \\ 124.89 \\ 17.907 \\ 22.134 \\ 55.321 \\ 22.363 \\ 17.842 \\ 189.87 \end{bmatrix}$$

$$Y223 := \begin{bmatrix} 100.07 \\ 23.844 \\ 18.88 \\ 124.89 \\ 182.26 \\ 22.222 \\ 55.634 \\ 22.453 \\ 18.158 \\ 189.9 \end{bmatrix}$$

20.215

20.412

20.317

$$NY232_{i} = \frac{Y232_{i}}{y_{c_{i}}}$$
  $NY221_{i} = \frac{Y221_{i}}{y_{c_{i}}}$   $NY223_{i} = \frac{Y223_{i}}{y_{c_{i}}}$ 

$$NY221_{i} = \frac{Y221}{y_{c_{i}}}$$

$$NY223_i := \frac{Y223_i}{y_{c_i}}$$

Evaluation of the Jacobi rnatrix

The three columns of the Jacobian are computed separately:

$$i := 0...NO - 1 \qquad A1_i := \frac{NY322_i - NY122_i}{Nx1_2 - Nx1_0} \quad A2_i := \frac{NY232_i - NY212_i}{Nx2_2 - Nx2_0} \quad A3_i := \frac{NY223_i - NY221_i}{Nx3_2 - Nx3_0}$$

then they will be augmented:

$$A := augment(A1,A2)$$
  $A := augment(A,A3)$ 

Construction of matrix W and vector b:

The standard form of the correlation matrix is created (see Report ), which represents the linearized balance equations.

$$W*Y-b=0$$

E := identity(11) W = augment(-A,E) 
$$b := Ny_c - A \cdot Nx_m$$

Construction of extended measurement vector Y<sub>m</sub>

This vector consists of the input and output variables:

Number of input variables: NI := 3

$$i := 0...NI - 1$$
  $NY_{m_i} := Nx_{m_i}$   $NY_{c_i} := Nx_{m_i}$   
 $i := NI...NO + NI - 1$   $NY_{m_i} := Ny_{m_{i-NI}}$   $NY_{c_i} := Ny_{c_{i-NI}}$ 

Generally, the measured values are not satisfied these balance equations:

Computing the error vector:

$$f := W \cdot NY_m - b$$

Construction of weight matrix, V

$$\begin{array}{lll} j := 0 ... \, NO + \, NI - \, 1 & i := 0 ... \, NO + \, NI - \, 1 & V_{i,j} := 0 \\ \\ i := 0 ... \, NI - \, 1 & V_{i,i} := \left(N\sigma_{X_i}\right)^2 & Z_{i,i} := \sigma_{X_i} \\ \\ i := \, NI ... \, NO + \, NI - \, 1 & V_{i,i} := \left(N\sigma_{Y_{i-NI}}\right)^2 & Z_{i,i} := \sigma_{Y_{i-NI}} \end{array}$$

The weigthed square of the error vector will be minimized under the constrain of the balance equations. The result will be the corrected values:

Number of freedom: F = NI

F = 3

 $\kappa^2$  distribution value at confidence p = 0.95 is: 7.815, see Mathematical Handbook for Scientists and Engineers, Korn & Korn, McGraw-Hill Co.

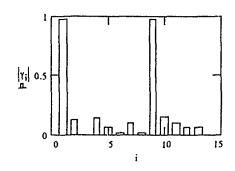
Because of Q > 7.815 we are looking for outliers, and compute the gamma index :

Computing Almásy gamma index:

$$i = 0.. NO + NI - 1$$

$$H := W^T \cdot \left(W \cdot V \cdot W^T\right)^{-1} \cdot W \qquad \quad h_i := \left(H_{i,i}\right)^{-\frac{1}{2}} \qquad \gamma := \frac{1}{q} \cdot \left[\operatorname{diag}(h) \cdot W^T \cdot \left(W \cdot V \cdot W^T\right)^{-1} \cdot f\right]$$

Almásy gamma



Conclusions: According to the statistical test, x2 input or y7 output is "wrong" measurement. It is pausable to vote for y7 and correct. The corrected value for y7 is the computed value.

Using this corrected value, 55.479 as "measured value" in vector y<sub>m</sub>, the result will show you that even now parameter estimation is necessary, because Q > 7.815

$$Y_{m_9} := 55.479$$
  $NY_{m_9} := \frac{Y_{m_9}}{y_{c_c}}$   $NY_{m_9} = 1$ 

$$NY_{m_9} := \frac{Y_{m_9}}{y_{c_c}}$$

#### **Parameter Estimation**

Linearization

The Jacobian matrix can be computed similarly, now we have five parameters instead of three input.

Construction of matrix B

$$p1 := \begin{pmatrix} 100 \\ 159.42 \\ 170 \end{pmatrix} \quad p2 := \begin{pmatrix} 30 \\ 38.29 \\ 50 \end{pmatrix} \qquad p3 := \begin{pmatrix} 60 \\ 81.577 \\ 100 \end{pmatrix} \qquad p4 := \begin{pmatrix} 1 \cdot 10^{-5} \\ 2.1 \cdot 10^{-5} \\ 3 \cdot 10^{-5} \end{pmatrix} \qquad p5 := \begin{pmatrix} 4 \cdot 10^{-5} \\ 6.3 \cdot 10^{-5} \\ 8 \cdot 10^{-5} \end{pmatrix}$$

$$i := 0... 2$$

$$Np1_{i} := \frac{p1_{i}}{p_{0}} \qquad Np2_{i} := \frac{p2_{i}}{p_{1}} \qquad Np3_{i} := \frac{p3_{i}}{p_{2}} \qquad Np4_{i} := \frac{p4_{i}}{p_{3}} \qquad Np5_{i} := \frac{p5_{i}}{p_{4}}$$

$$i := 0.. NO - 1$$

$$NY12222_{i} := \frac{Y12222_{i}}{y_{c_{i}}} \quad NY32222_{i} := \frac{Y32222_{i}}{y_{c_{i}}} \quad NY21222_{i} := \frac{Y21222_{i}}{y_{c_{i}}} \quad NY23222_{i} := \frac{Y23222_{i}}{y_{c_{i}}}$$

$$NY22122_{i} := \frac{Y22122_{i}}{y_{c_{i}}} \qquad NY22322_{i} := \frac{Y22322_{i}}{y_{c_{i}}} \qquad NY22212_{i} := \frac{Y22212_{i}}{y_{c_{i}}} \qquad NY22232_{i} := \frac{Y22232_{i}}{y_{c_{i}}}$$

$$NY22221_i := \frac{Y22221_i}{y_{c_i}}$$
  $NY22223_i := \frac{Y22223_i}{y_{c_i}}$ 

i := 0.. NO - 1

$$B1_{i} := \frac{NY32222_{i} - NY12222_{i}}{Np1_{2} - Np1_{0}} \qquad B2_{i} := \frac{NY23222_{i} - NY21222_{i}}{Np2_{2} - Np2_{0}} \qquad B3_{i} := \frac{NY22322_{i} - NY22122_{i}}{Np3_{2} - Np3_{0}}$$

$$B4_{i} := \frac{NY22232_{i} - NY22212_{i}}{Np4_{2} - Np4_{0}} \qquad B5_{i} := \frac{NY22223_{i} - NY22221_{i}}{Np5_{2} - Np5_{0}}$$

$$B = augment(B_1, B_2)$$
  $B = augment(B_1, B_3)$   $B = augment(B_1, B_3)$   $B = augment(B_1, B_3)$ 

$$j := 0...NI - 1$$
  $i := 0...NI + NO - 1$   $M_{i,j} := 0$   $S_{i,j} := 0$   $i := 0...NI - 1$   $M_{i,j} := 1$ 

$$i \coloneqq NI...NI + NO - 1 \qquad j \coloneqq 0...NI - 1 \qquad M_{i,j} \coloneqq A_{i \leftarrow NI,j}$$

Number of parameters: NP = 5

$$j := 0...NP - 1$$
  $S_{i,j} := B_{i-NI,j}$   $M := augment(M,S)$   $NdY := NY_m - NY_c$ 

Analysis of ridge regression  $\lambda > 0$ 

In order to get realistic results rigid regression can be used, because of the eigenvalues of the system matrix are too different :

$$\lambda := 1000$$

Eigenvalues of the original system matrix

Eigenvalues of the original modified system matrix

eigenvals 
$$(M^{T} \cdot V^{-1} \cdot M) = \begin{bmatrix} 1.248 \cdot 10^{14} \\ 1.978 \cdot 10^{5} \\ 8.076 \cdot 10^{4} \\ 1.809 \cdot 10^{3} \\ 968.285 \\ 0.675 \\ 8.534 \\ 139.471 \end{bmatrix}$$
 eigenvals  $(M^{T} \cdot V^{-1} \cdot M + \lambda \cdot identity(NI + NP)) = \begin{bmatrix} 1.248 \cdot 10^{14} \\ 1.988 \cdot 10^{5} \\ 8.176 \cdot 10^{4} \\ 2.809 \cdot 10^{3} \\ 1.968 \cdot 10^{3} \\ 1.001 \cdot 10^{3} \\ 1.009 \cdot 10^{3} \\ 1.139 \cdot 10^{3} \end{bmatrix}$ 

 $NdX := Isolve \left( M^{T} \cdot V^{-1} \cdot M + \lambda \cdot identity(NI + NP), M^{T} \cdot V^{-1} \cdot NdY \right)$ 

$$\begin{split} i &:= 0 ... NI + 1 & dX_i := NdX_i \cdot x_{m_i} \\ i &:= NI ... NI + NP + 1 & dX_i := NdX_i \cdot p_{i+NI} \end{split}$$

$$NdX = \begin{bmatrix} -4.574 \cdot 10^{-7} \\ -0.008 \\ -0.019 \\ 0.009 \\ 0.006 \\ -0.002 \\ 0.002 \\ -8.23 \cdot 10^{-4} \end{bmatrix}$$
Absolute corrections
$$dX = \begin{bmatrix} -1.087 \cdot 10^{-5} \\ -0.002 \\ -0.327 \\ 1.398 \\ 0.216 \\ -0.198 \\ 4.491 \cdot 10^{-8} \\ -5.185 \cdot 10^{-8} \end{bmatrix}$$

Even now, we have got negativ changes for the third and fifth parameters.

#### **Estimation without constrains**

New input values:

$$x1_e := x_{m_0} + dX_0$$
  $x2_e := x_{m_1} + dX_1$   $x3_e := x_{m_2} + dX_2$   $x1_e = 23.76$   $x2_e = 0.318$   $x3_e = 17.031$ 

New parameter values:

$$p1_{e} = p1_{1} + dX_{3}$$
  $p2_{e} = p2_{1} + dX_{4}$   $p3_{e} = p3_{1} + dX_{5}$   $p4_{e} = p4_{1} + dX_{6}$   $p5_{e} = p5_{1} + dX_{7}$ 

$$p := \begin{bmatrix} 159.42 \\ 38.29 \\ 81.577 \\ 2.1 \cdot 10^{-5} \\ 6.3 \cdot 10^{-5} \end{bmatrix}$$
 <-- Old parameters   
New parameters --> 
$$p_{e} = 160.818$$
$$p_{e} = 38.506$$
$$p_{e} = 81.379$$
$$p_{e} = 2.104 \cdot 10^{-5}$$
$$p_{e} = 6.295 \cdot 10^{-5}$$

In order to ensure, that the change in the parameters be positive, one can use estimation with constrains.

#### **Estimation with constrains**

From physical point of view the change in parameters must be positive (last five elements). In order to ensure that constrain is introduced, namely the change can not be negative. Introducing variable transformation,  $x \rightarrow x^2$ , minimization without constrains can be used.

$$G(\alpha,\beta,\gamma,\delta,\epsilon,\zeta,\eta,\theta) := \sum_{j=0}^{NI+NO-1} \frac{\left[NdY_{j} - \left(M_{j,0}\cdot\alpha + M_{j,1}\cdot\beta + M_{j,2}\cdot\gamma + M_{j,3}\cdot\delta^{2} + M_{j,4}\cdot\epsilon^{2} + M_{j,5}\cdot\zeta^{2} + M_{j,6}\cdot\eta^{2} + M_{j,7}\cdot\gamma + M_{j$$

For initial values the results of the estimation without constrains are employed if they were positive, and zeros were used in opposite cases. Use normalized values!

$$\alpha := 0.0$$
  $\beta := 0.0$   $\gamma := 0.0$   $\delta := \sqrt{\frac{1.398}{159.4}}$ 

$$\epsilon := \sqrt{\frac{0.216}{38.29}}$$
  $\zeta := 0.0$   $\eta := \sqrt{\frac{4.491 \cdot 10^{-8}}{2.1 \cdot 10^{-5}}}$   $\theta := 0.0$ 

Given

$$G(\alpha, \beta, \gamma, \delta, \epsilon, \zeta, \eta, \theta) = 0$$

|=|
|=|
|=|
|=|
|=|
|=|
|=|

$$w := Minerr(\alpha, \beta, \gamma, \delta, \epsilon, \zeta, \eta, \theta) \begin{bmatrix} 0 \\ 0 \\ 0.094 \\ 0.075 \\ 0 \\ 0.046 \\ 0 \end{bmatrix} \qquad NDX := \begin{bmatrix} w_0 \\ w_1 \\ w_2 \\ (w_3)^2 \\ (w_4)^2 \\ (w_5)^2 \\ (w_6)^2 \\ (w_7)^2 \end{bmatrix} \qquad NDX = \begin{bmatrix} 0 \\ 0 \\ 0.009 \\ 0.006 \\ 0 \\ 0.002 \\ 0 \end{bmatrix}$$

$$\begin{split} i &:= 0 ... NI - 1 & DX_i &:= NDX_{i'} x_{m_i} \\ i &:= NI ... NI + NP - 1 & DX_i &:= NDX_{i'} p_{i-NI} \end{split}$$

$$DX = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1.398 \\ 0.216 \\ 0 \\ 4.491 \cdot 10^{-8} \\ 0 \end{bmatrix}$$

New input values:

$$x1_{e} := x_{m_{0}} + DX_{0}$$
  $x2_{e} := x_{m_{1}} + DX_{1}$   $x3_{e} := x_{m_{2}} + DX_{2}$   $x1_{e} = 23.76$   $x2_{e} = 0.32$   $x3_{e} = 17.358$ 

New parameter values:

$$p1_{e} := p1_{1} + DX_{3} - p2_{e} := p2_{1} + DX_{4} - p3_{e} := p3_{1} + DX_{5} - p4_{e} := p4_{1} + DX_{6} - p5_{e} := p5_{1} + DX_{7} + DX_{8} - p5_{1} = p5_{1} + DX_{1} + DX_{2} + DX_{3} + DX_{4} + DX_{5} + DX_{5} + DX_{5} + DX_{5} + DX_{6} + DX_{6$$

Old parameters:

$$p = \begin{bmatrix} 159.42 \\ 38.29 \\ 81.577 \\ 2.1 \cdot 10^{-5} \\ 6.3 \cdot 10^{-5} \end{bmatrix}$$

$$p1_{e} = 160.818$$

$$p2_{e} = 38.506$$

$$p3_{e} = 81.577$$

$$p4_{e} = 2.104 \cdot 10^{-5}$$

$$p5_{e} = 6.3 \cdot 10^{-5}$$

Now on the bases of the new input values and new parameters, new output values can be computed by the PROBERA code, however no significant change took place in the parameter values.