Fuzzy model-based predictive control of a chemical reactor
Proceedings of European Congress of Chemical Engineering (ECCE-6)
Copenhagen, 16-20 September 2007

Fuzzy model-based predictive control of a chemical reactor

Anna Vasičkaninová, Monika Bakošová

Slovak University of Technology in Bratislava, Faculty of Chemical and Food Technology, Institute of Information Engineering, Automation and Mathematics, Radlinskeho 9, 812 37 Bratislava, Slovakia
e-mail: anna.vasickaninova@stuba.sk, monika.bakosova@stuba.sk

Abstract

Model-based predictive control (MBPC) refers to a class of control algorithms, which are based on a process model. MBPC can be applied to such systems as e.g. multivariable, non-minimum-phase, open-loop unstable, non-linear, or systems with a long time delay.
In this paper a comparison of different MBPC is presented as a case study for a continuous-time stirred reactor with two first-order irreversible parallel exothermic reactions. The focus is given to the fuzzy predictive control approach.
Chemical reactors with exothermic reactions represent the most dangerous operational units in the chemical industry. The temperature control is a real problem for conventional PID controllers in this case, and fuzzy MBPC is one of the possibilities how to solve it. In this approach, a fuzzy model gives a prediction of the plant output. The fuzzy predictive control approach is compared to a linear and nonlinear model predictive control based on an optimization. Simulation results show that fuzzy predictive control gives promising results.

Keywords: chemical reactor, fuzzy model, predictive control

1.Introduction

Nowadays, conventional controller techniques like PID solve with acceptable results most of the control problems in modern industry. However, to fulfill high-performance specifications dealing with constrained, multivariable and/or non linear systems, the process model must be included into the controller structure. MBPC has been well accepted in industry due to the generality of the method and a large number of industrial applications has already been introduced.
According to the process model two main approaches have been developed in the area of predictive control. The first one is based on a parametric model of the controlled process. The parametric model can be described in form of transfer function or in state-space domain. An important disadvantage of using the parametric model is that it represents a linearized model of the process. The control of the strong nonlinear processes could be unsatisfactory. The second approach proposed in literature is based on a nonparametric model. The model coefficients can

be obtained directly from samples of the input and output responses without assuming the model structure.
Predictive control is a control strategy that is based on the prediction of the plant output over the extended horizon in the future, which enables the controller to predict future changes of the measurement signal and to base control actions on the prediction.
The paper is organized as follows. Section 2 describes the concept of fuzzy identification. Section 3 presents the control strategy. In section 4 the continuous stirred-tank reactor is described, identification of the process in the fuzzy model form is obtained, simulation results and comparison of different MBPC control algorithms are presented and discussed. Finally, in section 5 some concluding remarks are presented.

2 Fuzzy modelling

Fuzzy modelling or identification means to find a set of fuzzy if-then rules with well defined attributes, that can describe the given I/O behaviour of the process.
Fuzzy modelling methods are attractive, because they can be developed from real process data with or without expert knowledge. The nonlinearity can be handled efficiently, and the results presented as fuzzy rules are informative. Many different approaches to fuzzy identification have been proposed. The most common alternatives are linguistic fuzzy models, which suit well extracting expert knowledge, neuro-fuzzy method and fuzzy clustering methods.
Fuzzy models can be considered as logical models, which use *If - Then* rules to establish qualitative relationships among variables in the model.

2.1 The fuzzy model

Consider the nonlinear plant in the form:

$$y(k+1)=F\{y(k),...,y(k-n+1),u(k),...,u(k-m+1)\} \tag{1}$$

where *y(k)* is the plant output at instance *k*, *F(.)* is a function, generally nonlinear, *u(k)* is an input signal. The constant *n* and *m* define the order of the plant. The Sugeno's of type the fuzzy model process can be formulated (Driankov 1993):

$$R^{i,j}:\ \ if\ y(k)\ is\ A_1^i \wedge u(k)\ is\ A_2^j\ \ then\ y_m(k+1)=\phi^{i,j}(.) \tag{2}$$

The functions $\phi^{i,j}(.)$ can be arbitrary smooth functions in general, although linear or affine functions are usually used. Each fuzzy set A_1^i, A_2^j is associated with a real-valued function $\mu(k)^{i,j}:\mathbb{R}\rightarrow[0,1]$, that produces membership grade of the variables *(y(k), u(k))*. Using fuzzy inference based upon product-sum-gravity at given input *(y(k), u(k))*, the final output of the fuzzy system is inferred by taking the weighted average of the $\phi^{i,j}(.)$'s:

$$y_m(k+1)=\frac{\sum_{i=1}^{N_i}\sum_{j=1}^{N_j}\mu(k)^{i,j}\phi^{i,j}(.)}{\sum_{i=1}^{N_i}\sum_{j=1}^{N_j}\mu(k)^{i,j}} \tag{3}$$

where $\mu(k)^{i,j}>0$, implies the overall truth value of the *i,j*-th implication for input calculated as:

$$\mu(k)^{i,j}=A_1^i(y(k))\times A_2^j(u(k)) \tag{4}$$

3. Model-based predictive control (MBPC)

MBPC is a name of a several different control techniques. All are associated with the same idea. The prediction is based on the model of the process.

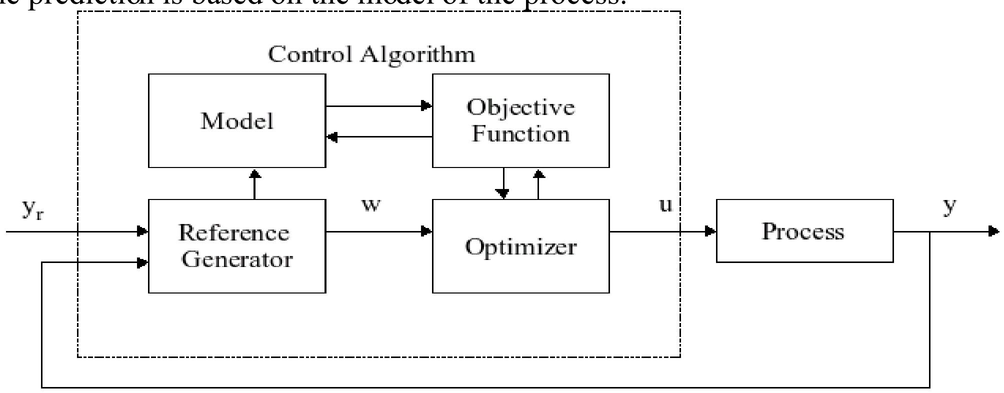

Figure 1: Classical model-based predictive scheme

The target of the model-based predictive control is to predict the future behaviour of the process over a certain horizon using the dynamic model and obtaining the control actions to minimize a certain criterion, generally

$$J(k,u(k))=\sum_{j=N_1}^{N_2}(y_m(k+j)-y_r(k+j))^2+\lambda\sum_{j=1}^{N_u}(u(k+j-1))^2 \tag{5}$$

Signals $y_m(k+j)$, $y_r(k+j)$, $u(k+j)$ are j-step ahead predictions of the process output, the reference trajektory and the control signal, respectively. The values N_1 and N_2 are minimal and maximal prediction horizon and N_u is prediction horizon of control signal. The parameter λ represents the weight of the control signal.
The controller consists of the plant model and the optimization block. The optimization block determines the value of u' that minimize J, and then the optimal u is input to the plant.
Equation (1) is used in combination with input and output constraints:

$$\begin{aligned} u_{min} &\leqslant u \leqslant u_{max} \\ \Delta u_{min} &\leqslant \Delta u \leqslant \Delta u_{max} \\ y_{min} &\leqslant y \leqslant y_{max} \\ \Delta y_{min} &\leqslant \Delta y \leqslant \Delta y_{max} \end{aligned} \tag{6}$$

4. Simulation results

4.1 Chemical reactor

Chemical reactors are ones of the most important plants in chemical industry (Mikleš and Fikar 2004). Consider a chemical reactor with first-order irreversible parallel reactions according to the scheme $A \xrightarrow{k_1} B \quad A \xrightarrow{k_2} C$. The measured outputs are concentrations of reactants and temperatures of reaction mixture and coolant. The simplified non-linear dynamic mathematical model of the chemical reactor consists of five differential equations:

$$\frac{dc_A}{dt}=\frac{q}{V}c_{Av}-\frac{q}{V}c_A-k_1c_A-k_2c_A \tag{7}$$

$$\frac{dc_B}{dt}=\frac{q}{V}c_{Bv}-\frac{q}{V}c_B+k_1c_A \tag{8}$$

$$\frac{dc_C}{dt}=\frac{q}{V}c_{Cv}-\frac{q}{V}c_C+k_2c_A \tag{9}$$

$$\frac{dT}{dt}=\frac{q}{V}T_v-\frac{q}{V}T-\frac{Ak}{V\rho C_p}[T-T_c]-\frac{\dot{Q}_r}{V\rho C_p} \tag{10}$$

$$\frac{dT_c}{dt}=\frac{q_c}{V_c}T_{vc}-\frac{q_c}{V_c}T_c+\frac{Ak}{V_c\rho_c C_{pc}}[T-T_c] \tag{11}$$

The reaction rate coefficients are non-linear functions of reaction temperatures being defined by the Arrhenius relations

$$k_1=k_{10}e^{-\frac{E_1}{RT}} \qquad k_2=k_{20}e^{-\frac{E_2}{RT}} \tag{12}$$

The reaction heat is expressedas

$$\dot{Q}_r=k_1c_AV(\Delta_rH_1)+k_2c_AV(\Delta_rH_2) \tag{13}$$

Here, c are concentrations, T are temperatures, V are volumes, r are densities, C_P are specific heat capacities, q are volumetric flow rates, Δ_rH are reaction enthalpies, A is the heat transfer area, k is the heat transfer coefficient. The subscript c denotes the coolant, and the subscript s the steady-state values in the main operating point. Parameters and inputs of the reactor are enumerated in Table 1.

Variable	Unit	Value
q	m^3min^{-1}	0.015
v	m^3	0.23
V_C	m^3	0.21
ρ	kg m^{-3}	1020
ρ_C	kg m^{-3}	998
C_p	kJ kg K^{-1}	4.02
C_{pc}	kJ kg K^{-1}	4.182
A	m^2	1.51
k	kJ m^2 min^{-1} K^{-1}	42.8
k_{10}	min^{-1}	$1.55.10^{11}$
k_{20}	min^{-1}	$4.55.10^{25}$
E_1/R	K	9850
E_2/R	K	22019
Δ_rH_1	kJ $kmol^{-1}$	$-8.6.10^4$
Δ_rH_2	kJ kmol-1	$-1.82.10^4$
c_{Av}	kmol m^{-3}	4.22
c_{Bv}	kmol m^{-3}	0

Variable	Unit	Value
c_{Cv}	kmol m-3	0
T_v	K	328
T_{cv}	K	298
q^s_c	m^3min^{-1}	0.004
T^s	K	363.61
Ts_c	K	350.15
c^s_A	kmol m^{-3}	0.4915
c^s_B	kmol m^{-3}	2.0042
c^s_C	kmol m^{-3}	1.7243

Table 1: Reactor parameters and inputs

Consider the linearized model of the CSTR in the form (14) with matrices ***A**, **B**, **C***:

$$\begin{aligned}\dot{\boldsymbol{x}}(t) &= \boldsymbol{A}\boldsymbol{x}(t) + \boldsymbol{B}\boldsymbol{u}(t), \qquad \boldsymbol{x}(t_0)=\boldsymbol{x_0}\\ \boldsymbol{y}(t)&=\boldsymbol{C}\boldsymbol{x}(t)\end{aligned} \tag{14}$$

$$\boldsymbol{A} = \begin{bmatrix} -\left(\frac{q}{V}+k_{11}+k_{21}\right) & 0 & 0 & -\left(k_{12}+k_{22}\right) & 0 \\ k_{11} & -\frac{q}{V} & 0 & k_{12} & 0 \\ k_{21} & 0 & -\frac{q}{V} & k_{22} & 0 \\ -\left(\frac{k_{11}\Delta_r H_1+k_{21}\Delta_r H_2}{\rho C_p}\right) & 0 & 0 & -\left(\frac{q}{V}+\frac{A\ k}{V\rho C_p}+\frac{k_{12}\Delta_r H_1+k_{22}\Delta_r H_2}{\rho C_p}\right) & \left(\frac{A\ k}{V\rho C_p}\right) \\ 0 & 0 & 0 & \left(\frac{A\ k}{V_c\rho_c C_{pc}}\right) & -\left(\frac{A\ k}{V_c\rho_c C_{pc}}+\frac{q^s_c}{V_c}\right) \end{bmatrix} \tag{15}$$

$$\boldsymbol{B} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \frac{T_{cv}-T^s_c}{V_c} \end{bmatrix} \qquad \boldsymbol{C} = \begin{bmatrix} 0 & 0 & 0 & 1 & 0 \end{bmatrix}$$

where

$$\begin{aligned} k_{11}&=k_{10}e^{-\frac{E_1}{RT^s}} \qquad & k_{12}&=\frac{c^s_A E_1}{R(T^s)^2}k_{10}e^{-\frac{E_1}{RT^s}}\\ k_{21}&=k_{20}e^{-\frac{E_2}{RT^s}} \qquad & k_{22}&=\frac{c^s_A E_2}{R(T^s)^2}k_{20}e^{-\frac{E_2}{RT^s}} \end{aligned} \tag{16}$$

Linearized mathematical model of the reactor has been derived under assumption that the control input is the coolant flow rate q_c and the controlled output is reaction mixture temperature T.

For applications of linear MBP controller, we consider model in the form

$$\boldsymbol{x}(k+1) = \boldsymbol{A}\boldsymbol{x}(k) + \boldsymbol{B}\boldsymbol{u}(k)$$
$$\boldsymbol{y}(k) = \boldsymbol{C}\boldsymbol{x}(k) \tag{17}$$

where matrices $\boldsymbol{A}$, $\boldsymbol{B}$ are:

$$\boldsymbol{A} = \begin{bmatrix} -0.5594 & 0 & 0 & -0.0284 & 0 \\ 0.2662 & -0.0652 & 0 & 0.0098 & 0 \\ 0.2280 & 0 & -0.0652 & 0.0187 & 0 \\ 6.5956 & 0 & 0 & -0.1538 & 0.0685 \\ 0 & 0 & 0 & 0.0737 & -0.0928 \end{bmatrix} \quad \boldsymbol{B} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ -248.2571 \end{bmatrix} \tag{18}$$

Fuzzy identification is an effective tool for the approximation of uncertain nonlinear systems on the basis of measured data. Among the different fuzzy modelling techniques, the Takagi-Sugeno model has attracted most attention.

In the case of the reactor fuzzy model, the process was identified in a form of discrete model with the premise $T(k)$ and the consequence vector $[T(k), T(k-1), q_c(k)]$. The structure with five rules and Gaussian membership functions was chosen. The sampling time was chosen to be $T_s = 0.2\ min$. The structure of the fuzzy model is given:

$$\begin{aligned} &\mathit{if}\ T(k)\ \mathit{is}\ A_1 \wedge T(k-1)\ \mathit{is}\ A_2\ \wedge q_c(k)\ \mathit{is}\ A_3 \\ &\mathit{then}\, T(k+1) = a_{1i}T(k) + a_{2i}T(k-1) + b_{1i}q_c(k) + b_{0i}, \quad i=1,\ldots,5 \end{aligned} \tag{19}$$

The Gaussian membership functions premise parameters σ_i, c_i for inputs are listed in Table 2, the rules consequent parameters are listed in Table 3. The Takagi-Sugeno fuzzy model was transformed into a state space form.

T(k)		*T(k-1)*		q_c	
σ_i	c_i	σ_i	c_i	σ_i	c_i
0.331	363.601	0.331	363.601	-0.0003	0.0040
0.331	357.182	0.331	357.109	0.0019	0.0091
0.331	353.426	0.331	353.423	0.0099	0.0112
0.331	356.059	0.331	356.054	-0.0014	0.0101
0.331	366.577	0.331	366.587	0.0002	0.0020

Table 2 - Gaussian membership functions parameters for inputs

a_{1i}	a_{2i}	b_{1i}	b_{0i}
2.21	-1.22	-19.5	3.64
2.21	-1.22	-23.97	4.21
2.07	-1.07	-10.39	-0.90
2.07	-1.08	-4.19	3.73
2.04	-1.04	-0.0003	-0.17

Table 3 - Rules consequent parameters

A comparison of the nonlinear and linearized model output with the Takagi-Sugeno fuzzy model output is shown in Figure 2.

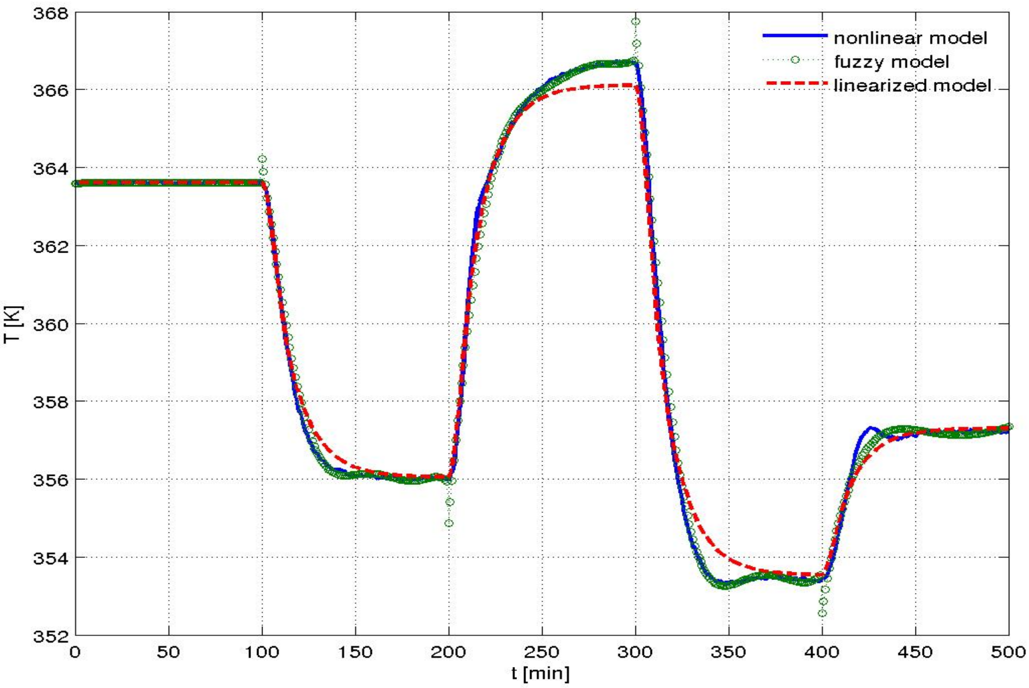

Figure 2: Simulated outputs of the plant models

4.2 Comparison of different MBPC control algorithms

The reactions in the described reactor are exothermic and the heat generated by the chemical reaction is removed by the coolant. The control objective is to keep reactant temperature close to a desired value.

An important difference between Model Predictive Control and PID-kind design methods is the explicit use of a model. This aspect is both the advantage and the disadvantage of MPC.

Nonlinear model based predictive control, fuzzy model based predictive control and linear based model predictive control have been simulated and compared with same conditions. Finally, the comparison with a PID controller was made. The feedback PID controller was tuned with parameters $K_C = -0.003$, $T_I = 16.8$, $T_D=1.41$ using the Chien-Hrones-Reswick method (Bakošová 2004, Ogunnaike 1994, Vasičkaninová 2005).

In Figure 3 the responses of the process and the reference trajectory y_r are shown. Simulation results show that fuzzy predictive control gives promising results.

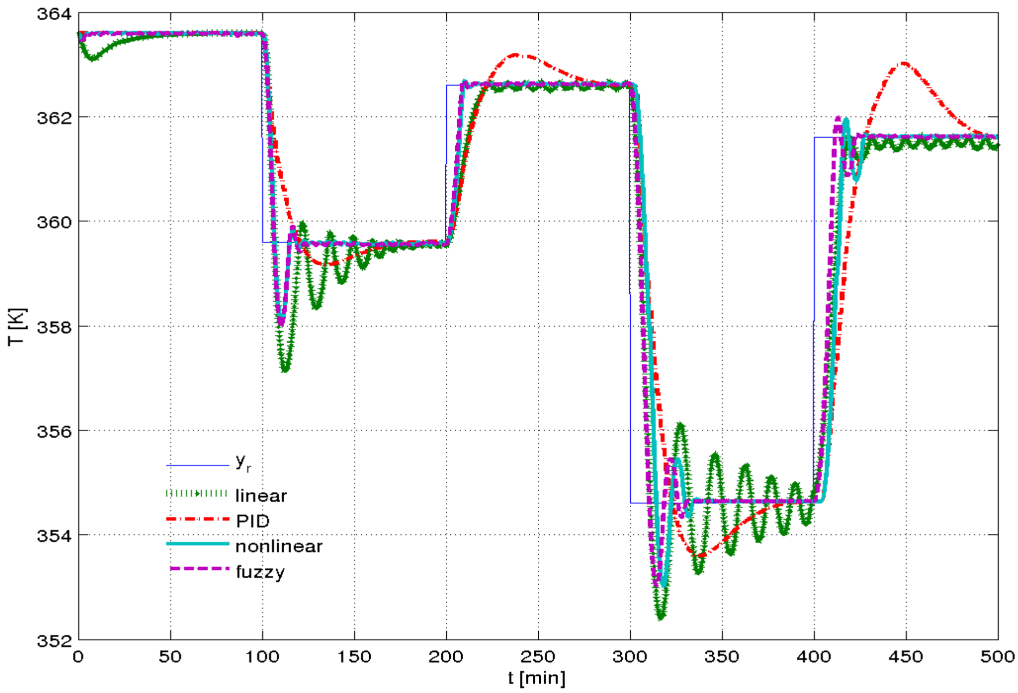

Figure 3: Comparison of chosen model based predictive control simulations with PID controller.

5. Conclusion

The predictive controllers are used in many areas, where high-quality control is required. In the paper the predictive controller for the well-known process, the continuous stirred tank reactor is presented. The focus is given to the fuzzy predictive control approach. The Takagi-Sugeno fuzzy model of the reactor was obtained using fuzzy identification. Comparing to PID, it improved quality and robustness performance.

Acknowledgments

The authors are pleased to acknowledge the financial support of the Scientific Grant Agency of the Slovak Republic under grants No. 1/3081/06 a 1/4055/07.

References

Bakošová, M., Vasičkaninová, A., Karšaiová, M., and Ondrovičová, M., PID controller tuning for cascade control of a chemical reactor. In: *Proc. 6. International Scientific-Technical Conf. Process Control 2004.* Kouty nad Desnou. University of Pardubice, p. 63. ISBN 80-7194-662-1, (2004).

Driankov, D., Helerndoorn, H., *An Introduction to Fuzzy Control*, Springer-Verlag, Berlin, (1993).

Georgescu, C., Afshari, A. and Bornard, G., Fuzzy predictive PID controllers: An eating control application, *2th IEEE Conference on Fuzzy System,* 1091- 1098, (1993).

Jang, S. R., Adaptive-Network-Based Fuzzy Inference Systems, IEEE Trans. Systems, Man & Cybernetics 23, 665-685, (1993).

Mikleş J. and M. Fikar (2004). Process modelling, identification and control II. STU Press, Bratislava.

Morari, M., and Zafiriou, F., *Robust Process Control.* Chapter, Prentice-Hall, (1989).

Nauck, D., Klawonn, F., and Kruse, R., *Foundations of neuro-fuzzy systems.* John Wiley & Sons, Great Britain. Able, B.C. (1956). Nucleic acid content of microscope. *Nature* 135, 7-9, (1997).

Ogunnaike, B. A. and Ray, W. H., *Process Dynamics, Modelling, and Control.* 536-541. Oxford University Press. New York. 1259. ISBN 0-19-509119-1, (1994).

Passino, K. M., Yurkovich, S., *Fuzzy Control*, Addison-Wesley, California, (1998).

Rivera, D. E., Morari, M., and Skogestad, M., Internal Model Control, *4. PID Controller Design, and Eng. Proc. Des. Dev.,* 23., (1986).

Roubos, J. A., Mollov, S., Babuška, R. and Verbruggen, H. B., Fuzzy model-based predictive control using Takagi-Sugeno models, *International Journal of Approximate Reasoning* 22, 3-30, (1999).

Sugeno, M., and Yasukawa, T., *A fuzzy logic approach to qualitative modelling*. IEEE trans. FS, 1, 1,7-31, (1993).

Vasičkaninová, A., and Bakošová, M., Cascade fuzzy logic control of a chemical reactor. V *Proc. 15. Int. Conference Process Control '05*, Štrbské Pleso, High Tatras, (2005).