SLOVAK UNIVERSITY OF TECHNOLOGY IN BRATISLAVA

Faculty of Electrical Engineering and Information Technology

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Dissertation Thesis Abstract

Hybrid Predictive Control Approach Based on Soft Computing Methods

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ABSTRACT

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FACULTY OF ELECTRICAL ENGINEERING AND INFORMATION TECHNOLOGY

Study program:	5.2.14 Automation and Control
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The dissertation thesis deals with the hybrid MPC control design for a nonlinear chemical reactor. Based on the analysis of nonlinear processes and applied control methods in the chemical and petrochemical industries, an innovative solution to the control problem using a hybrid controller is developed. The controller is based on neural networks to predict and model non-measurable states. A solution to the discrete states in a hybrid prediction model with discrete sub-model switching is proposed. The thesis provides a deep insight into the kinetic modelling of the specific chemical reaction. It is shown that the mathematical modelling of the kinetic process during the polymerization reaction is generally applicable in the control theory. An application of the kinetic model for MPC of a highly nonlinear process with discrete states is developed. Advantages and disadvantages of the conventional mathematical and the hybrid modelling approaches are assessed. Reactor and plant operation data used in the thesis were acquired from a real polypropylene unit operated in a petrochemical company.

Key words: Hybrid, Nonlinear, Model Predictive Control, Polypropylene, Soft-Control

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SÚHRN

SLOVENSKÁ TECHNICKÁ UNIVERZITA V BRATISLAVE

FAKULTA ELEKTROTECHNIKY A INFORMATIKY

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Dizertačná práca:	Hybridné prediktívne riadenie s využitím inteligentných výpočtových metód

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Dizertačná práca sa zaoberám návrhom riadenia hybridného MPC pre nelineárny chemický reaktor. Na základe analýzy nelineárneho procesu a aplikovaných metód riadenia v chemickom a petrochemickom priemysle bolo vyvinuté inovatívne riešenie problému riadenia použitím hybridného regulátora. Na predikciu a modelovanie nemerateľných stavov sú v regulátore použité neurónové siete. Diskrétne stavy v hybridnom predikčnom modeli sú riešené prepínaním diskrétnych submodelov.

Predložená dizertačná práca poskytuje detailnú analýzu kinetického modelovania chemickej reakcie polymerizácie. Je ukázané, že matematické modelovanie kinetického procesu polymerizácie je všeobecne použiteľné v teórii riadenia. Kinetický model je využitý v štruktúre MPC pre proces polymerizácie pre vysoko nelineárny proces s diskrétnymi stavmi. Porovnané sú výhody a nevýhody konvenčného matematického modelovania a hybridného modelovania. Údaje o prevádzke reaktorov použité v práci boli získané zo skutočnej polypropylénovej jednotky prevádzkovanej v existujúcej petrochemickej spoločnosti.

Kľúčové slová: Nelineárne systémy, model, prediktívne riadenie, Polypropylén, inteligentné metódy

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1. Dissertation Thesis objectives

The aim of the dissertation is to analyze the possibility of implementing modified advanced control in a petrochemical plant, and to develop an appropriate control method based on soft computing approaches (neural networks). The process selected is a polypropylene reactor Rx1 in the polypropylene plant PP5 in a Slovak petrochemical company. This plant uses an Advanced Process Control system provided by the technology licensor, and the method behind this system is intellectual property of the APC company. However, actual process data have been provided by the plant operator to complete this thesis. The dissertation thesis outline was proposed as follows:

1. Analysis of nonlinear processes in a selected area of the chemical industry.
2. Design of advanced control methods for a nonlinear chemical process using MPC and soft computing strategies.
3. Verification of the proposed control methods and algorithms for the nonlinear polypropylene fluidized bed reactor.
4. Comparison of advanced and conventional control methods and algorithms
5. Comparison of the proposed hybrid methodology with the existing advanced control strategies in chemical industry

Analysis of selected nonlinear processes in the chemical and petrochemical industry and applied control methods are provided in the Introduction. Along with an overview of possible neural network architectures in the first chapter it completes the introduction to this main topic. The chapter Problem formulation explains and defines the fundamental problems and provides a deep insight into the MPC strategy and neural network used in combination with this approach. The chapter Case study provides a complete description of the control problem, proposed solution and verification of methods proposed for the selected process. In the final chapter, a comparison of the results achieved using the proposed and the conventional methods is presented. In the chapter Conclusion the achieved results have been assessed and compared. The achieved results and philosophical achievements of the proposed methodology are pointed out in the chapter – Achievements.

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2. Introduction to the modeling and control

Continuously increasing the computational power and capacity of new processors is an opportunity which is exploited also in the field of industry and industrial control systems. Thanks to the continuous improvement of the computational capacity of the resources there are new fields opening in the area of control system development. Transition from 16 to 32 and finally to 64-bit instruction set, together with continuously increased capacity and power, means that the new methodologies may be implemented. [1] The control methods used in the industry is varying according to industry type. However, the mostly used technology is PID algorithm. [1] Only several types of different basic algorithms are used, which are modified according to the need of particular application (environment, processor type, unification). To these requirements belong time delay of the controlled process and specific process dynamics.

2.1. Nonlinear systems and control – an overview

In industrial applications is the problem is usually solved by linearization of the process the ar operating point. This approach is then limiting the plant operation range and increasing the effort required to operate the plant within the broader range. Approaching the problem with a nonlinear control structure may solve this limitation and provide higher flexibility to the plant operator. Many chemical processes are designed conservatively to avoid complex operating regimes. Coordination of design, operation, and control optimization is necessary to prevent overdesign. Therefore, the methods described later in this chapter make operation at optimal economic conditions a realistic goal.

2.1.1. Model predictive control

The MPC technology offers advantages where the others are facing a disadvantage. This technology provides optimal control while respecting the constraints. The second advantage related to the mentioned problems is applying MPC technology to the nonlinear control tasks. The MPC technology offers the highly valued feature of implementation constraints in the controller design, which helps to operate the process efficiently near the plant limits, prevents damage to the equipment, and increases the operation's safety. In most cases, the MPC ensures a more complete and optimal solution than other common approaches, which leads to the controller being "tuned" to a lowest standard denominator solution that is stable under all plant conditions but is optimal for none. Model uncertainty and process disturbances are handled by calculating an additive disturbance as the difference between the process measurement and the model prediction at the current time step. It is assumed that the future disturbances are equal to the present disturbance, and a new trajectory is then calculated.

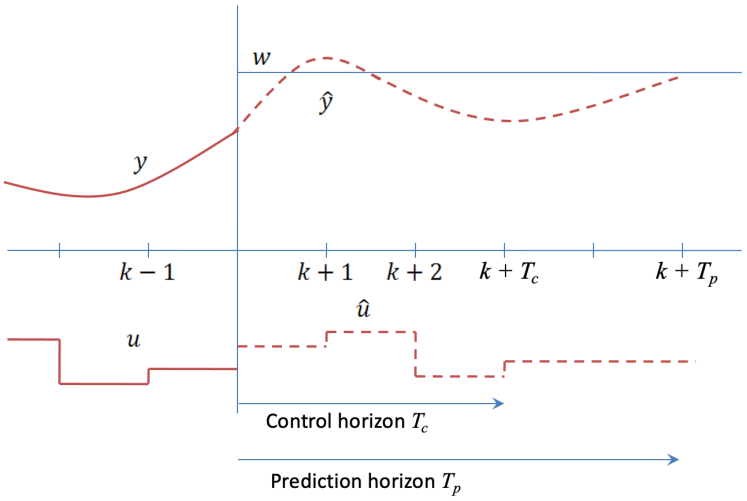

Figure 1: Predictive control method

The industry has well-received predictive control strategies because they are intuitive and explicitly handle constraints. A limitation to the conventional MPC methods is that they are based on linear systems theory and may not perform well on highly nonlinear systems. An obvious extension of the linear MPC methods is when a nonlinear dynamic process model is used instead of a linear convolution model. The objective of nonlinear model predictive control

(NLMPC) is to calculate a set of future control moves within the control horizon to minimize a function based on the desired output trajectory over a prediction horizon. Graphical expression of the MPC method we show in *Figure 1*.

2.2. Neural networks in nonlinear control

Neural networks are considered universal approximators. Therefore, many researchers have been working to implement this strategy into the conventional control methods. Functionality and flexibility of neural networks will allow conventional methods to leverage the advantages of neural networks while suppressing the conventional view's disadvantages. The following chapter presents a brief theoretical overview and introduction to neural network technology.

2.2.1. Process control based on neural networks review

For most applications, first principles models are the preferable choice, mainly when applied with process control methodologies [2]. The disadvantage of using the first-principle models is that these models are challenging to maintain as the parameters change with time. Large and distributed systems could be challenging to obtain or identify the first-principle models [2]. Thanks to machine learning, the neural networks fit the input and output data using the internal or hidden layers as universal approximators. The disadvantage of neural networks as system models is their lack of physical knowledge in their formulation.

2.2.2. Neural observer for nonlinear systems

The MPC uses the model of process to compute the future manipulations according to current states of the process/model. The future manipulations are a result of optimization of the control move according to current model states. Therefore, the knowledge of the current states is absolutely necessary for the MPC algorithm. Generally, the state variables are hard to measure, depending on the type of the process which is an object of control. The states have to be computed or estimated using the input and output data of the controlled system [3]. The functional control block used for process state reconstruction is called an observer or state estimator. The main function of the observer, estimator, or sometimes called as filter, is to reconstruct the current state according to past inputs and outputs.

2.2.3. ANN state observer

Another structure which uses the neural network technology is the control method based on system state observation by an observer, which is providing the information about the internal process state according to the process input and output variables. [4] The general structure of the observer-based control structure is shown in Figure 2.

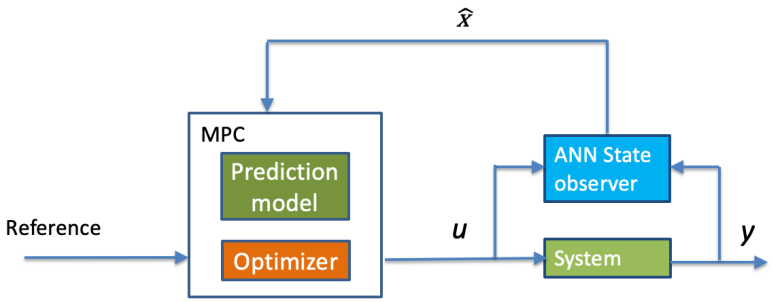

Figure 2: Control structure with external state observer

3. The polypropylene production

This work's primary target and purpose are to analyze the possible application of hybrid MPC methods based on the soft computing approach in the industry. The method's application has been simulated and analyzed using the real process data from an existing plant. The process selected for this task is common and essential in the petrochemical industry – polymerization in fluidized bed reactor. This process is nonlinear, affected by many inputs and having several internal state variables. Polymerization reactor is usually online almost entire year and primarily operated in optimal conditions developed by long term operation. However, the natural advantages of the optimal constrained control method provided by the MPC method may improve optimal plant operation. Even a small improvement of operating condition may provide significant improvement in asset value. The problem related to this topic can be divided into several sub-problems.

- Process analysis - First of all, a detailed understanding of the technology was necessary to ensure causality and selection of essential data for system identification. Because we will be designing a control system for the central production unit, we will focus on production rate control. A necessary step in the research is to understand all inputs and technology subsystems that significantly affect polymerization production.
- Data processing - Another challenging problem is to analyze the data and finding appropriate tools and methods for processing and preparing the data for the system identification and simulation experiments.
- Simulation and development environment - Consideration of the development environment and setup is another important milestone for the research. Because we will not conduct experiments with an actual unit in production, a setting for control system design and validation has been selected.
- System identification - Development and validation of simulation model and design of scenarios for the model validation and control system development. Although system identification is an essential step in this research, the main focus will be to control method development and validation.
- Control method development – The aim of dissertation thesis is to develop a method of hybrid control method based on optimal MPC for highly nonlinear process. The nonlinear behavior of the process has been investigated and modeled using the neural networks. Validation criteria has been designed and performance different approaches evaluated.

The data used during the thesis are downloaded from an existing plant after decades of operation. A set of data provided by the plant operator is one full year. As-built documentation has also been provided for the research, which is subject to a non-disclosure agreement. However, the as-built has to be considered with a reserved approach because the polypropylene plant underwent several reconstruction and renewal projects. Therefore, the original reactor parameters slightly changed over time.

3.1. UNIPOL process description

The process selected for this work is a worldwide well-known and frequently used process - the Union Carbide gas-phase polypropylene process (UNIPOL). The UNIPOL process is a result of cooperation between Union Carbide Corporation and Shell chemical [6]. This work focused on the central part of the process: the homopolymer system part (Figure 3). The UNIPOL process is based on a chemical reaction in a reactor bed fluidized by a large volume of gas flowing through the reactor. This gas provides three main functions, which are mixing, heat removal, and temperature control. Heat removal is an essential point of consideration because polymerization is an exothermic reaction. Our case's heat removal is ensured by cycle gas cooled down in a cycle gas cooler unit. In the latest literature [5] can be found that the heat removal can be partially substituted by some amount of liquid evaporation in the fluidized bed. This principle is frequently called the condensation mode type of cooling.

In the reactor, a reaction occurs in the gas phase in the Ziegler – Natta catalyst. The gas stream provides monomer (C3H6), hydrogen (H2), and Catalyst (Ziegler-Natta) to the reactor. These are the precursors and variable costs – as much as you use, that much is produced. Anyway, there is a couple of parameters that directly or indirectly affect the reaction rate. Cycle gas feed stream fluidizes and agitates the reactor bed and removes the polymerization reaction's heat. Since the reaction occurs in the gas phase, reactor pressure is an important parameter. The temperature of the reaction is one of the critical parameters. The reaction occurs in the pores of Ziegler – Natta catalyst and the presence of co-catalyst together with selectivity control agent. The catalyst suspension is created according to the catalyst manufacturer's datasheet and recipe before reactor injection in a separate system. Therefore, the catalyst is considered

as a single stream input. The non-reacted gas leaves the top of the reactor, is processed, cooled, and then returned to the system.

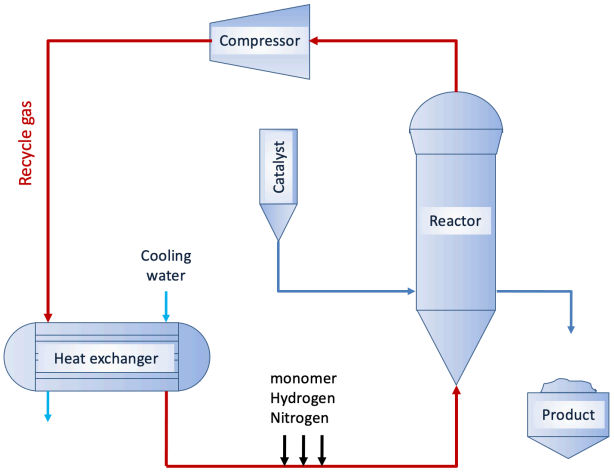

Figure 3: UNIPOL system basic principle

3.2. Plant data

The research's initial and essential requirement was that the designed control method should be evaluated and validated with actual process data from an existing plant. The data for this study has been provided by a petrochemical company Slovnaft a.s.. The data have been recorded during one year of operation of polypropylene unit PP5. The data have been recorded in the year 2014 and fully represent operational parameters, inputs, and outputs. The data have been provided in Excel sheets as tables with a sampling period of 30 minutes and another set with 1 minute. According to the discussion with plant representatives, these values are average values. Deep analysis has been carried out with these data because it contains values of different kinds and different accuracy.

3.3. System identification

It is essential to keep in mind that polymerization reaction modeling is a complex problem and the fact that this work also focused on control system development and validation. Therefore, simplification has been considered during the system identification and modeling. The UNIPOL process technology comprises several different subsystems. The main element and also point of interest of this study is the main reactor where the polymerization occurs. The reaction itself occurs in the pores of the catalyst particles.

3.3.1. Terminology and symbols used in the model

In the following section and tables are explanations of symbols and values used in the reaction model. In Table 1 are variables, values, and symbols used in the reaction model.

Table 1: Nomenclature and used symbols in polymerization reactor model

Variable	Explanation	Variable	Explanation
V_{FB}	Fluidized bed volume $V_{FB} = \pi . r_{Rx1}^2 . h_{FB} . (1 - \varepsilon_{mf})$ $[m^3]$	T_{ref}	Reference temperature $[K]$
$C_a(t)$	The molar concentration of catalyst particles in reactor $[mol.m^{-3}]$	$M_{in}^{C2}(t)$	Ethylene mass flow rate into the reactor $[kg.h^{-1}]$
$F_{in}^{Ca}(t)$	Catalyst volume flow rate into the reactor $[m^3.h^{-1}]$	$\rho_{C2}(t)$	Ethylene density $[kg.m^{-3}]$
$Cat(i)$	The molar concentration of catalyst particles at reactor inlet $[mol.m^{-3}]$	$M_{in}^{H2}(t)$	Hydrogen mass flow rate into the reactor $[kg.h^{-1}]$
$k_a(t,i)$	The activation reaction rate constant $[s^{-1}]$	$\rho_{H2}(t)$	Hydrogen density $[kg.m^{-3}]$

$v_{SGV}(t)$	Superficial gas velocity $[m.s^{-1}]$	M_w^{C3}	The molecular weight of propylene $[kg.kmol^1]$
$h_{FB}(t)$	The actual level of fluidized-bed $[m]$	M_w^{C2}	The molecular weight of ethylene $[kg.kmol^1]$
$C_{C3}(t)$	The molar concentration of propylene in reactor $[mol.m^{-3}]$	M_w^{H2}	The molecular weight of hydrogen $[kg.kmol^1]$
$F_{in}^{C3}(t)$	Propylene volume flow rate into the reactor $[m^3.h^{-1}]$	$P_1(t)$	Active site concentration with the length of 1 $[mol.m^{-3}]$
C_{in}^{C3}	The molar concentration of propylene at reactor inlet $[mol.m^{-3}]$	$P_l(t)$	Active site concentration with the length of l $[mol.m^{-3}]$
$F_{out}^{CG}(t)$	Cycle gas volume flow $[m^3.s^{-1}]$	T_{ret}	Reactor retention time $[s]$
$k_{im}(t,i)$	Initiation by propylene reaction rate constant $[m^3.mol^{-1}.s^{-1}]$	$Y_1(t)$	The first moment of living polymer chains $[mol.m^{-3}]$
$P_0(t)$	Active site concentration $[mol.m^{-3}]$	$Y_2(t)$	The second moment of living polymer chains $[mol.m^{-3}]$
$k_p(t,i)$	Propagation by monomer reaction rate constant $[m^3.mol^{-1}.s^{-1}]$	$X_0(t)$	0-th moment of dead polymer chains $[mol.m^{-3}]$
$Y_0(t)$	0-th moment of living polymer chains $[mol.m^{-3}]$	$X_1(t)$	The first moment of dead polymer chains $[mol.m^{-3}]$
$k_{fm}(t,i)$	Transfer to propylene reaction rate constant $[m^3.mol^{-1}.s^{-1}]$	$X_2(t)$	The second moment of dead polymer chains $[mol.m^{-3}]$
$C_{C2}(t)$	The molar concentration of ethylene in reactor $[mol.m^{-3}]$	c_p^{PP}	Specific heat capacity of polypropylene at 342 K $[J.mol^{-1}.K^{-1}]$
$F_{in}^{C2}(t)$	Ethylene volume flow rate into the reactor $[m^3.h^{-1}]$	$\rho_{PP}(t)$	Polypropylene density $[kg.m^{-3}]$
C_{in}^{C2}	The molar concentration of ethylene at reactor inlet $[mol.m^{-3}]$	$T(t)$	The temperature in the reactor $[K]$
$k_{ic}(t,i)$	Initiation by ethylene reaction rate constant $[m^3.mol^{-1}.s^{-1}]$	$\tilde{\rho}_{CG}(t,i)$	Cycle gas specific gravity $[kg.m^{-3}]$
$k_{pc}(t,i)$	Propagation by ethylene reaction rate constant $[m^3.mol^{-1}.s^{-1}]$	T_{in}	Cycle gas temperature at the reactor inlet $[K]$
$k_{fcm}(t,i)$	Transfer to ethylene reaction rate constant $[m^3.mol^{-1}.s^{-1}]$	A_{FB}	Cycle gas to fluidized bed heat transfer coefficient
$C_{H2}(t)$	The molar concentration of hydrogen in reactor $[mol.m^{-3}]$	$-H^d(i)$	The heat of reaction – deactivation $[J.mol^{-1}]$
$F_{in}^{H2}(t)$	Hydrogen volume flow rate into the reactor $[m^3.s^{-1}]$	$+H^{im}(i)$	The heat of reaction – initiation by propylene $[J.mol^{-1}]$
C_{in}^{H2}	The molar concentration of hydrogen at reactor inlet $[mol.m^{-3}]$	$+H^{icm}(i)$	The heat of reaction – initiation by ethylene $[J.mol^{-1}]$
$k_H(t,i)$	Transfer to hydrogen reaction rate constant $[m^3.mol^{-1}.s^{-1}]$	$+H^H(i)$	The heat of reaction – transfer to hydrogen $[J.mol^{-1}]$
$M_{in}^{Ca}(t)$	Catalyst mass flow rate into the reactor $[kg.h^{-1}]$	$+H^{fm}(i)$	The heat of reaction – transfer to propylene $[J.mol^{-1}]$
ρ_{Ca}	Catalyst suspension density $[kg.m^{-3}]$	$+H^{fcm}(i)$	The heat of reaction – transfer to ethylene $[J.mol^{-1}]$
$M_{in}^{C3}(t)$	Propylene mass flow rate into the reactor $[kg.h^{-1}]$	$-H^{dI}(i)$	The heat of reaction –reaction poisoning $[J.mol^{-1}]$
$\rho_{C3}(t)$	Propylene density $[kg.m^{-3}]$	$+H^p(i)$	The heat of reaction –propagation by propylene block $[J.mol^{-1}]$
p_{Rx1}	Reactor gas cap pressure $[bar]$	$+H^{pc}(i)$	The heat of reaction –propagation by ethylene block $[J.mol^{-1}]$
p_{atm}	Atmospheric pressure $[bar]$	ε_{mf}	The void fraction at minimum fluidization [-]
T_{atm}	Atmospheric temperature $[K]$	$\rho_{H2}(t)$	Hydrogen density $[kg.m^{-3}]$

3.3.2. Reaction kinetics

Reaction kinetics is a part of physical chemistry that is concerned with understanding the rates of chemical reactions. It contrasts to thermodynamics, which deals with the direction in which a process occurs but in itself tells nothing

about reaction rates. For a quantitative and qualitative description of the process, we have to focus on the chemical reaction. The polymerization reaction is a sequence of elementary steps which can be described as

1. Activation
   The titanium chloride compound has a crystal structure in which each Ti atom is coordinated to chlorine atoms.
2. Initiation step
   The formation of the alkene-metal complex initiates the polymerization process. In our case, the alkene monomer is gaseous propylene, and the metal atom is provided by the ZN catalyst – Titanium.
3. Chain propagation step
   The propagation step is a straightforward phase of the reaction which, under specific conditions, repeats and the polymer molecular weight increases.
4. Chain termination step
   Termination is the last and final phase of a polymer chain growth. There are multiple reasons for the chain termination.

3.3.3. Reaction rate and reaction kinetics

Each chemical reaction somehow depends on the temperature at which the reaction takes place. The best way how to express the chemical reaction depending on temperature is exactly through reaction rate. In physical chemistry, the formula which describes the temperature dependence of reaction rates is called the Arrhenius equation.

In modeling chemical processes, we recognize the chemical reaction of different orders. According to the number of reagents, the chemical reaction order is started according to a simplified principle. An irreversible chemical reaction where a reagent A is transferred into a product B is shown in Equation 1.

$$A \xrightarrow{k} B \tag{1}$$

In Equation 1 the k is the kinetic rate constant. In reaction described by Equation 1, one mol of reactant A produces one mol of product B (a stoichiometric reaction). The reaction rate gives the speed of reaction.

The summary state reaction kinetics equations are

$$V_{FB}.\frac{dC_a(t)}{dt} = F_{in}^{Ca}(t).Cat(i) - k_a(t,i).\left(C_a(t) + \frac{v_{SGV}}{h_{FB}}\right) \tag{2}$$

$$V_{FB}.\frac{dC_{C3}(t)}{dt} = F_{in}^{C3}(t).C_{in}^{C3} - F_{out}^{CG}(t).C_{C3}(t) - C_{C3}(t).\left(k_{im}(t,i).P_0(t) + k_p(t,i).Y_0(t) + k_{fm}(t,i).Y_0(t)\right) \tag{3}$$

$$V_{FB}.\frac{dC_{C2}(t)}{dt} = F_{in}^{C2}(t).C_{in}^{C2} - F_{out}^{CG}(t).C_{C2}(t) - C_{C2}(t).\left(k_{ic}(t,i).P_0(t) + k_{pc}(t,i).Y_0(t) + k_{fcm}(t,i).Y_0(t)\right) \tag{4}$$

$$V_{FB}.\frac{dC_{H2}(t)}{dt} = F_{in}^{H2}(t).C_{in}^{H2} - F_{out}^{CG}(t).C_{H2}(t) - C_{H2}(t).(k_H(t,i).Y_0(t)) \tag{5}$$

$$V_{FB}.\frac{dP_0(t)}{dt} = k_a(t,i).C_a(t) - P_0(t).\left(k_{im}(t,i).C_{C3}(t) + k_{ic}(t,i).C_{C2}(t) + \frac{v_{SGV}}{h_{FB}}\right) \tag{6}$$

$$V_{FB}.\frac{dY_0(t)}{dt} = P_0(t).\left(k_p(t,i).C_{C3}(t) + k_{pc}(t,i).C_{C2}(t)\right) - Y_0(t).\left(k_{fm}(t,i).C_{C3}(t) + k_{fcm}(t,i).C_{C2}(t) + k_H(t,i).C_{H2}(t) + \frac{v_{SGV}}{h_{FB}}\right) \tag{7}$$

$$V_{FB}.\frac{dY_1(t)}{dt} = P_0(t).\left(k_p(t,i).C_{C3}(t) + k_{pc}(t,i).C_{C2}(t)\right) + Y_0(t).\left(k_{fm}(t,i).C_{C3}(t) + k_{fcm}(t,i).C_{C2}(t)\right) + Y_0(t).\left(k_p(t,i).C_{C3}(t) + k_{pc}(t,i).C_{C2}(t)\right) - Y_1(t).\left(k_{fm}(t,i).C_{C3}(t) + k_{fcm}(t,i).C_{C2}(t) + k_H(t,i).C_{H2}(t) + \frac{v_{SGV}}{h_{FB}}\right) \quad (8)$$

$$V_{FB}.\frac{dY_2(t)}{dt} = P_0(t).\left(k_p(t,i).C_{C3}(t) + k_{pc}(t,i).C_{C2}(t)\right) + Y_0(t).\left(k_{fm}(t,i).C_{C3}(t) + k_{fcm}(t,i).C_{C2}(t)\right) + \left(2.Y_0(t) + Y_0(t)\right).\left(k_p(t,i).C_{C3}(t) + k_{pc}(t,i).C_{C2}(t)\right) - Y_2(t).\left(k_{fm}(t,i).C_{C3}(t) + k_{fcm}(t,i).C_{C2}(t) + k_H(t,i).C_{H2}(t) + \frac{v_{SGV}}{h_{FB}}\right) \quad (9)$$

$$V_{FB}.\frac{dX_0(t)}{dt} = Y_0(t).\left(k_{fm}(t,i).C_{C3}(t) + k_{fcm}(t,i).C_{C2}(t) + k_H(t,i).C_{H2}(t)\right) - X_0(t).\left(\frac{v_{SGV}}{h_{FB}}\right) \quad (10)$$

$$V_{FB}.\frac{dX_1(t)}{dt} = Y_1(t).\left(k_{fm}(t,i).C_{C3}(t) + k_{fcm}(t,i).C_{C2}(t) + k_H(t,i).C_{H2}(t)\right) - X_1(t).\left(\frac{v_{SGV}}{h_{FB}}\right) \quad (11)$$

$$V_{FB}.\frac{dX_2(t)}{dt} = Y_2(t).\left(k_{fm}(t,i).C_{C3}(t) + k_{fcm}(t,i).C_{C2}(t) + k_H(t,i).C_{H2}(t)\right) - X_2(t).\left(\frac{v_{SGV}}{h_{FB}}\right) \quad (12)$$

3.3.4. Material and energy balance

In this work, we will describe the group, which is the continuous stirred tank reactor (CSTR). The reason for selecting the CSTR type of reactor is that the UNIPOL technology with fluidized bed reactor is similar to this type of reactor. In CSTR, the reactants and products are continuously fed in and out to/from the reactor. The cycle gas ensures the delivery of the reactant and the mixing and fluidization of the reactor bed. With these definitions, the CSTR type of reactor is the best candidate for the reactor approximation and model design. [7] Due to the nature of material delivery, product withdraws, and energy distribution, the type of reactor is critical for physical properties modeling and material and energy balances. For the thesis, it is only required to have a complete view of the reactor production. Therefore, it is sufficient for work purposes to consider the reactor as a system with lumped parameters rather than the system with distributed parameters. While kinetic modeling is important for understanding the chemical reaction and effect of each reactant on the production rate, physical reaction modeling and consecutive equations of fluid flow represent mathematical description and statements of the conservation of mass, known as the equation of continuity. The resulting state energy balance equation is

$$V_{FB}.c_p^{PP}.\rho_{PP}(t)\frac{dT}{dt} = F_{out}^{CG}.\tilde{\rho}_{CG}(t,i).c_p^{CG}.(T_{in} - T) + V_{FB}.A_{FB}.(T_{in} - T) + V_{FB}.\left[k_d(t,i).I_d(t).P_0(t).(-H^d(i)) + k_{im}(t,i).P_0(t).C_{C3}(t).(+H^{im}(i)) + k_{icm}(t,i).P_0(t).C_{C2}(t).(+H^{icm}(i)) + k_H(t,i).Y_0(t).C_{H2}(t).(+H^H(i)) + k_{fm}(t,i).Y_0(t).C_{C3}(t).(+H^{fm}(i)) + k_{fcm}(t,i).Y_0(t).C_{C2}(t).(+H^{fcm}(i)) + k_d(t,i).Y_0(t).(-H^d(i)) + k_{dI}(t,i).Y_0(t).I_d(t).(-H^{dI}(i)) + k_p(t,i).Y_0(t).C_{C3}(t).(+H^p(i)) + k_{pc}(t,i).Y_0(t).C_{C2}(t).(+H^{pc}(i))\right] \quad (13)$$

3.3.1. The production rate

The production rate and the model output function is defined as

$$y(t) = R = M_{wC3}.\left[C_{C3}.Y_0(t).k_p(i)\right] + M_{wC2}.\left[C_{C2}.Y_0(t).k_{pc}(i)\right], \quad for\ i = 1,2\ or\ 3 \quad (14)$$

The process state vector is defined as

$$\boldsymbol{x}(t) = [C_a, C_{C3}, C_{C2}, C_{H2}, P_0, Y_0, Y_1, Y_2, X_0, X_1, X_2, T]^T \quad (15)$$

And the input vector defined as

$$\boldsymbol{u}(t) = [F_{in}^{Ca}, F_{in}^{C3}, F_{in}^{C2}, F_{in}^{H2}, T_{in}, v_{SGV}, h_{FB}, p_{Rx1}, \rho_{C3}, \rho_{C2}, \rho_{H2}, \rho_{PP}, i]^T \quad (16)$$

3.3.1. Product switching – hybrid system

The product types change often, but according to plant specification and operational parameters, there are thirteen different product types produced in total. The catalyst is then sprayed into the reactor, and polypropylene is produced in required quantities. According to the discrete product type state, the switching between the products is discrete, as shown in Figure 4. The product type condition is a part of state variables and has three different discrete states. According to product type state variable, the product-specific rate constants and enthalpies are selected together with catalyst density.

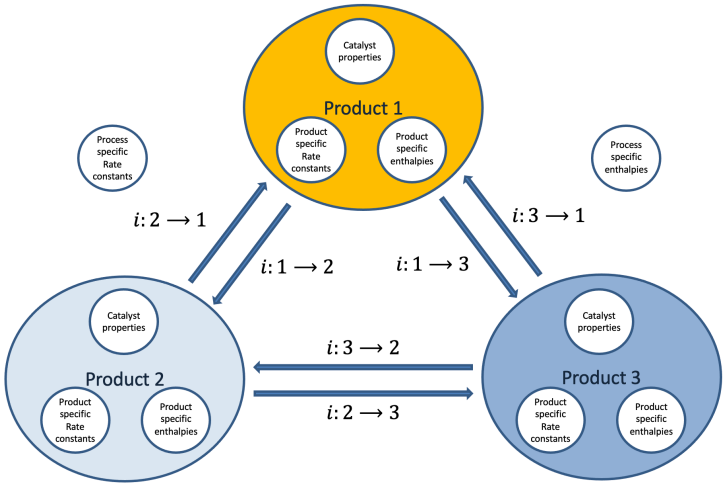

Figure 4: Discrete state diagram of product switching

The simulation model of the process is then defined as

$$\dot{\boldsymbol{x}}(t) = \begin{cases} \boldsymbol{f}_1(\boldsymbol{x}(t), \boldsymbol{u}(t)), & for\ i = 1 \\ \boldsymbol{f}_2(\boldsymbol{x}(t), \boldsymbol{u}(t)), & for\ i = 2 \\ \boldsymbol{f}_3(\boldsymbol{x}(t), \boldsymbol{u}(t)), & for\ i = 3 \end{cases} \quad (17)$$
$$, \boldsymbol{x}(0) = \boldsymbol{x}_0\ and\ \boldsymbol{u}(0) = \boldsymbol{u}_0$$

This means that the product type is the one additional input to the system. The output variable is defined as

$$y(t) = \begin{cases} \boldsymbol{g}_1(\boldsymbol{x}(t)), & for\ i = 1 \\ \boldsymbol{g}_2(\boldsymbol{x}(t)), & for\ i = 2 \\ \boldsymbol{g}_3(\boldsymbol{x}(t)), & for\ i = 3 \end{cases} \quad (18)$$
$$, \mathbf{x}(0) = \mathbf{x}_0$$

While Equation 14, 17 and 18 are valid for

$$\begin{aligned} &y(t) \in R, \forall t \geq 0 \\ &\boldsymbol{u}(t) \in U, \forall t \geq 0 \\ &\boldsymbol{x}(t) \in X, \forall t \geq 0, \end{aligned} \quad (19)$$

where the state vector is defined as $\boldsymbol{x}(t) \in \mathbb{R}^{12}$ and manipulated variable defined as $\boldsymbol{u}(t) \in \mathbb{R}^{13}$, while we are interested only in one output variable defined over $\mathrm{y}(t) \in \mathbb{R}^{1}$. The sets R, *U,* and *X* are specified as follows

$$\begin{aligned} R &:= \{y(t) \in \mathbb{R}^1 | y_{min} \leq y \leq y_{max}\} \\ U &:= \{\boldsymbol{u}(t) \in \mathbb{R}^{13} | \boldsymbol{u}_{min} \leq \boldsymbol{u} \leq \boldsymbol{u}_{max}\} \\ X &:= \{\boldsymbol{x}(t) \in \mathbb{R}^{12} | \boldsymbol{x}_{min} \leq \boldsymbol{x} \leq \boldsymbol{x}_{max}\} \end{aligned} \quad (20)$$

where 13-th input vector dimension means the product type and vectors $\boldsymbol{u}_{min}$, $\boldsymbol{u}_{max}$, $\boldsymbol{x}_{min}$ and $\boldsymbol{x}_{max}$ are physical or technological constraints of the plant. The values $\mathrm{y}_{\mathrm{min}}$ and $\mathrm{y}_{\mathrm{max}}$ are physical and safety constraints to the output

variable. The product type stands for the discrete state and thus switching between functions $\mathbf{f}_1$, $\mathbf{f}_2$ and $\mathbf{f}_3$ and $\mathbf{g}_1$, $\mathbf{g}_2$ and $\mathbf{g}_3$. Although the real system does have some physical constraints and is subject to limitations, these will be considered in the controller.

3.4. Control system design

The dissertation thesis main target is to research advanced control methods. Fitting the physical constants of the identified simulation model to the real data acquired from the existing plant gives good preconditions for considering that the situations tested in the simulation are close to the real situation at the plant. The actual plant runs and is controlled by the existing Advanced Process Control (APC) control system, provided with UNIPOL license. Predictive control system with the implementation of the hybrid technologies, together with increasing computational resources, is the subject of this thesis. Model predictive and intelligent or hybrid systems are suitable for nonlinear system control. The polymerization process is a nonlinear process with multiple states and variables. The UNIPOL process is a widely used technology globally, and effective and optimal control is the point of heavy interest.

3.4.1. Hybrid models

Process models are developed to describe the behavior of a process of any kind of interest. The models can be of various types beginning with the mathematical model, represented by partial or ordinary differential equations, and ending with physical or conceptual models. The mathematical formulation is oriented to signify the essential physical properties of the process. However, mathematical formulations may be difficult or even impossible to have in required accuracy or information level. The difficulties with mathematical formulations are hidden in numerous aspects like time dependency, nonlinearity, discontinuity, etc. The fundamental classification of models is related to the architecture of the relation by which the model transforms input to the output.

The mathematical model and model performance are based on knowledge about the process and process data we can measure. Based on these, we recognize three different classes of models, which are shown in Figure 5.

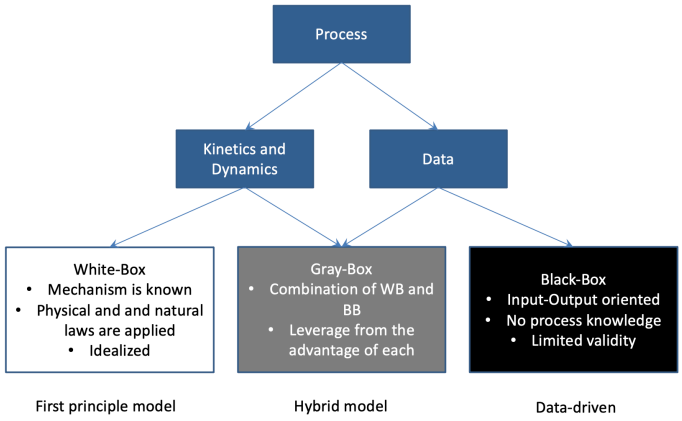

Figure 5: Mathematical models depending on process knowledge and data

The white-box model or also called the first-principle model, is based on first principle laws and dependencies. Physical laws give the mathematical structure, and their dependence on data shall be minimal. These models rely on precise knowledge of the process mechanism and offer maximum transparency to the model [8].

Black-box models are data-driven models that do not rely on process knowledge but only on mapping the input versus output. Examples of a black-box model are neural networks or fuzzy models.

The gray-box or hybrid models represent a combination of the two approaches described above. The advantages of both limit approaches may be systematically mixed to maximize the leverage of each. The effective hybrid modeling strategy results in a final model, where the black-box sub-model compensates shortcomings of the white-box modeling approach. Common sub-models like fuzzy models or neural networks may be combined in various structures to form a hybrid model with the required capabilities. Chemical reactor offers multiple points where the BB and WB mixed modeling approach is suitable for process control.

3.4.2. Hybrid control method using the neural approach

The polypropylene reaction kinetics modeling approach proposed includes several theoretical state variables which are not possible to measure and are necessary for selected control method application [9,10,11,12]. The reaction kinetics modeling approach used in this study introduces the method of moments for polymer chain distributions. These reaction moments are then used to estimate the product production rate. The reaction moments are theoretical values and are not measurable. However, during the experiments with the process data, it appears necessary to use them for future process output prediction. The mixed gray-box (GB) modeling approach is proposed in this work as a possible way to introduce the unmeasurable process states to the prediction model by a trained neural network.

3.4.3. Measurable and unmeasurable state feedback

We investigate two types of feedback variables measurable state variables, which are physical values that can measure with the transmitter, like concentrations, pressure, flow, or bed height. The other type of feedback variables are virtual states related to the reaction kinetics. It is not possible to measure these variables. In this thesis, we propose using a neural network for the feedback estimation of the state variables, which are virtual and therefore not measurable by any measuring device. The measurement of the polymer production rate would be possible, with some extra effort. However, having the chemical reaction kinetic modeled also brings advantages related to the final product quality information.

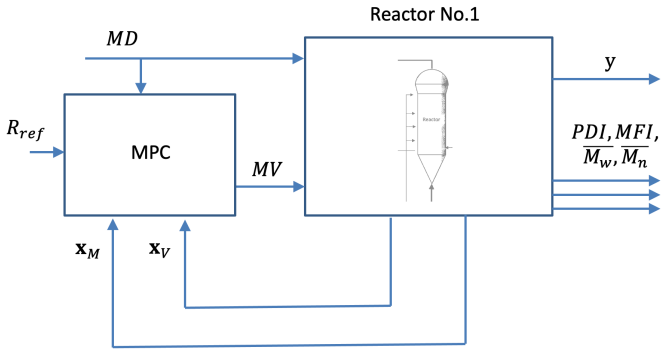

Figure 6: Measurable and unmeasurable process feedback

In Figure 6Figure 6, the state feedback is separated into two groups of variables. One of them is physical variables which are measured with no issues also in the real plant. The variables $\mathbf{x}_M(\mathrm{t}) = [\mathrm{C_a}, \mathrm{C_{C3}}, \mathrm{C_{C2}}, \mathrm{C_{H2}}, \mathrm{T}]^{\mathrm{T}}$ and $\mathbf{x}_V(\mathrm{t}) = [\mathrm{P_0}, \mathrm{Y_0}]^{\mathrm{T}}$ represent the feedback states. The state vectors' particular variables represent the molar concentrations of the reactants $\mathrm{C_a}, \mathrm{C_{C3}}, \mathrm{C_{C2}}, \mathrm{C_{H2}}$ The temperature at which the reaction occurs T. Due to the significant cycle gas flow, the molar concentration is in plant measured at the reactor outlet, upstream the cycle gas compressor. The second vector $\mathbf{x}_V(\mathrm{t})$ represent the unmeasurable state vector, which stands for virtual molar concentrations of the initiated active catalyst sites and living polymer chains. Unmeasurable variables $\mathrm{P_0}$ and $\mathrm{Y_0}$ provide information about the actual polymer chain length distribution and the zero-th moment of the chain length.

MPC strategy has been selected as the best candidate for the conventional control strategy, and combination with the neural network has been studied. The neural network has been used as a universal approximator to supplement the function of the process model. For this purpose, a Nonlinear Autoregressive neural network with exogenous input – NARX has been selected due to the conservative approach and known application with accessible programming tools.

3.4.1. Nonlinear MPC

Nonlinear MPC calculates control actions at each control interval using a combination of model-based constrained optimization. The prediction model is nonlinear. For our particular case of the polymerization reactor, the prediction model may be reduced to the number of states necessary for production rate calculation. Since a nonlinear MPC controller is a discrete-time controller and the state function is continuous-time, the model gets discretized by the controller using the implicit trapezoidal rule. This method was considered as sufficiently accurate and provide satisfactory prediction according to simulation results. This method approximates the integration over an interval by breaking the area down into trapezoids with more easily computable areas. For example, in Figure 7 is a trapezoidal integration of the sine function using the trapezoids.

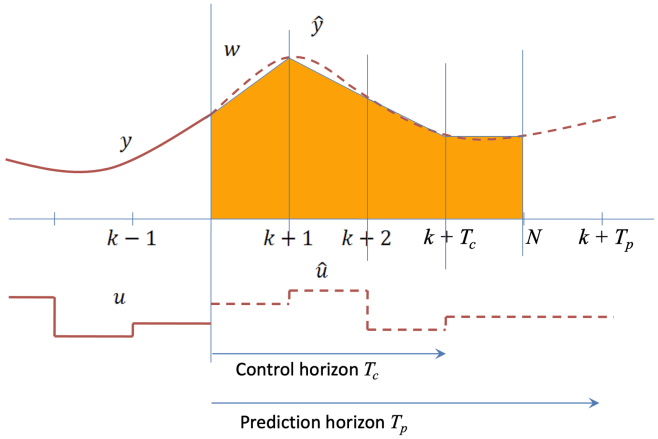

Figure 7: Trapezoidal discretization method

As manipulated variable was selected, the catalyst feed. While considering the other reactants' amount, the more catalyst is added to the system, the more polypropylene the plant produces. In Figure 8 is shown a block structure of the model, which has three inputs and one output. First input MV represents the manipulated variable, MD_C stands for continuous and MD_D for discrete inputs. For the MPC controller, these inputs MD_C and MD_D represent measurable disturbances and provide additional input information for the prediction model. The part of the cycle is consumed for the reaction and all of this occurs continuously. More catalyst is supplied to the system as the manipulated variable. The polymer production consumes more reactants. When more reactions occur inside the reactor, more heat is generated, and more heat needs to be removed. Otherwise, the pellets will start to coagulate, and the reactor will need a shutdown.

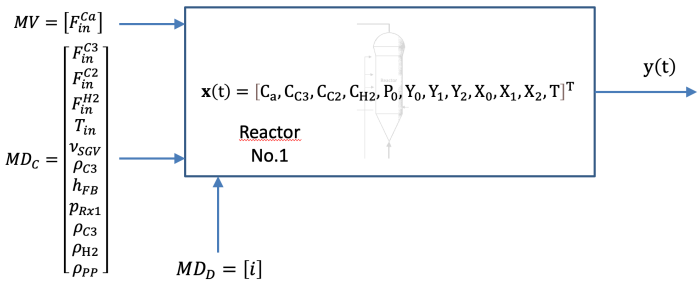

Figure 8: Simulation model structure, inputs, and outputs

In Figure 8 is shown a general overview of the simulation model structure. The output from the simulation model $\mathrm{y(t)}$ is the production rate $(t.h^{-1})$. The simulation model has 12 dynamic states, representing the reactant concentrations, polymer chain distribution, living and dead polymer chain distribution moments $(mol.m^{-3})$. and reactor interior temperature (K). The discrete input i represents the product type currently produced and provides information to the model, which model parameters to use.

The control problem is complex, and therefore an accurate prediction of output is required. The prediction model proposed uses all states that affect the production rate and all the states needed to consider all aspects properly. Catalyst dosage to the reactor as a manipulated variable seems to be trivial, but the state variables' consequences are complex.

3.4.2. Hybrid prediction model

The model and controller's hybridization can be found in two different layers and levels. One level is the request for control of a hybrid system with discrete and continuous states. The other level of hybridization is the controller topology. In this thesis, we propose using a neural network for the feedback estimation of the state variables, which are virtual and therefore not measurable by any measuring device. The state feedback is separated into two groups of variables. One of them is physical variables which are measured with no issues also in the real plant. The variables $\mathbf{x}_M(\mathrm{t}) = [\mathrm{C_a}, \mathrm{C_{C3}}, \mathrm{C_{C2}}, \mathrm{C_{H2}}, \mathrm{T}]^{\mathrm{T}}$ and $\mathbf{x}_V(\mathrm{t}) = [\mathrm{P_0}, \mathrm{Y_0}]^{\mathrm{T}}$ represent the feedback states. The state vectors' particular variables represent the molar concentrations of the reactants $\mathrm{C_a}, \mathrm{C_{C3}}, \mathrm{C_{C2}}, \mathrm{C_{H2}}$ The temperature at which the reaction

occurs T. Due to the significant cycle gas flow, the molar concentration is in plant measured at the reactor outlet, upstream the cycle gas compressor. The second vector $\mathbf{x}_V(t)$ represent the unmeasurable state vector, which stands for virtual molar concentrations of the initiated active catalyst sites and living polymer chains.

The measurable state variables are

$$\boldsymbol{x}_M(t) = [C_a, C_{C3}, C_{C2}, C_{H2}, T]^T \tag{21}$$

The estimated state variables which are not measurable are expressed

$$\hat{\boldsymbol{x}}_V(t) = \left[\hat{P}_0, \hat{Y}_0\right]^T \tag{22}$$

The estimated rate of polymer production, and the molecular weight increase, are then dependent only on the rate of advancement of the zeroth moment.

$$\hat{y}(t) = \hat{R} = M_{wC3}.\left[C_{C3}.\hat{Y}_0(t).k_p(i)\right] + M_{wC2}.\left[C_{C2}.\hat{Y}_0(t).k_{pc}(i)\right], \quad for\ i = 1{,}2\ or\ 3 \tag{23}$$

where the state vector is defined as $\boldsymbol{x}(t) \in \mathbb{R}^7$ and manipulated variable defined as $\boldsymbol{u}(t) \in \mathbb{R}^{13}$,

$$\boldsymbol{u}(t) = [F_{in}^{Ca}, F_{in}^{C3}, F_{in}^{C2}, F_{in}^{H2}, T_{in}, v_{SGV}, h_{FB}, p_{Rx1}, \rho_{C3}, \rho_{C2}, \rho_{H2}, \rho_{PP}, i]^T \tag{24}$$

while we are interested only in one output variable defined over $\mathrm{y}(t) \in \mathbb{R}^1$. The sets R, U and X are specified as follows

$$\begin{aligned} R &:= \{y(t) \in \mathbb{R}^1 | y_{min} \le y \le y_{max}\} \\ U &:= \left\{ \begin{matrix} \boldsymbol{u}(t) \in \mathbb{R}^{13} | \boldsymbol{u}_{min} \le \boldsymbol{u} \le \boldsymbol{u}_{max}, \\ \Delta u_{min}(1) \le \Delta u(1) \le \Delta u_{max}(1) \end{matrix} \right\} \\ X &:= \{\boldsymbol{x}(t) \in \mathbb{R}^{12} | \boldsymbol{x}_{min} \le \boldsymbol{x} \le \boldsymbol{x}_{max}\} \end{aligned} \tag{25}$$

where y_{min}, y_{max}, $\boldsymbol{x}_{min}, \boldsymbol{x}_{max}, \boldsymbol{u}_{min}, \boldsymbol{u}_{max}$ and $\Delta \mathrm{u}_{\min}(1)$ and $\Delta \mathrm{u}_{\max}(1)$ are physical and operational constraints of the variables.

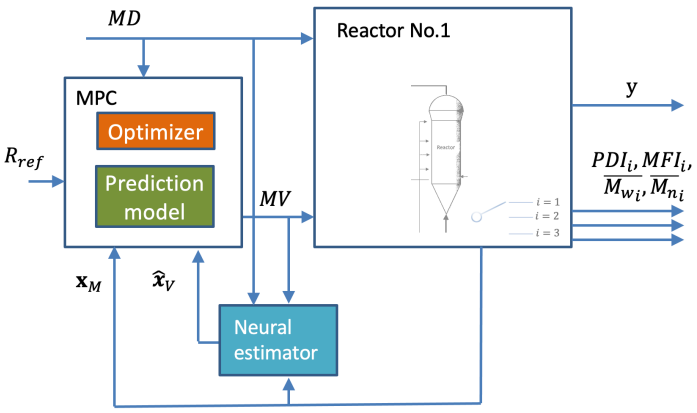

Figure 9: Simulation model structure with MPC and neural estimator

In Figure 9 is shown the control structure with a neural estimator for the unmeasurable state variables. The effect of the measurement noise on the measurable values has been simulated, and the robustness of the system response to them has been presented on the simulated trends. The designed MLP's and the overall prediction model structure are shown in the figures below.

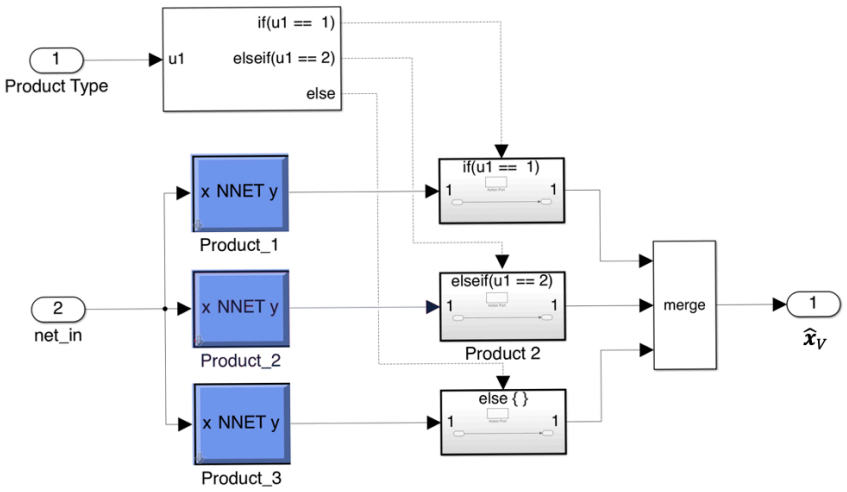

Figure 10: Prediction model with different MLP for particular product types, designed in MATLAB

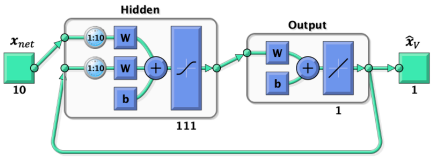

Figure 11: Dedicated MLP for Product 1

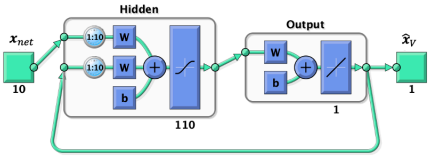

Figure 12: Dedicated MLP for Product 2

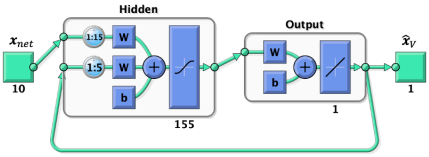

Figure 13: Dedicated MLP for Product 3

To observe the effect of the MLP structure on the prediction performance, the MLP dedicated to Product 3 has a slightly different topology than the MLP for Product 1 and 2. Controller and optimization constraints

$$R := \{y(t) \in \mathbb{R}^1 | 0\ t.h^{-1} \leq y \leq 50\ t.h^{-1}\}$$
$$U := \{-2\ kg.h^{-1} \leq \Delta u \leq 2\ kg.h^{-1}\} \quad (26)$$
$$X := \{\boldsymbol{x}(t) \in \mathbb{R}^{12} | -\infty \leq \boldsymbol{x} \leq \infty\}$$

4. Conclusion

Comparison between mathematical model and model based on neural network state estimator gives the result as expected. The control structure using the mathematical model for output prediction shows performance better than the neural network alternative. According to the selected criteria, the difference is about 7 – 14 % better results from the mathematical option than the neural network alternative. This difference is principal and natural to the soft computing technologies and the numerical accuracy of the neural network tools in the used computational environment – Matlab. The comparison between the mathematical and neural model with three dedicated neural networks is shown in Figure 14.

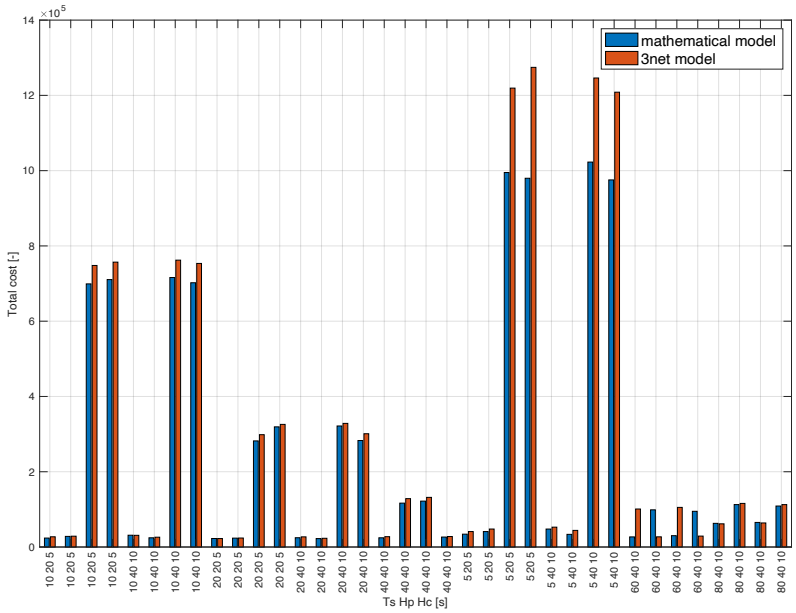

Figure 14: Mathematical and neural network prediction performance comparison

In Figure 14 is visible that in few alternatives of sampling period and control and prediction horizon shows the neural network version (3net) better performance than the mathematical version. Axis X represents variations of Ts – sampling period, Hp – prediction horizon, and Hc – control horizon of the MPC. The total cost is calculated as the sum of all qualitative parameters. It is shown on axis Y. Lower value means better performance, shorter time for execution, or less energy needed by the manipulator.

Another critical view on the control quality is the reference tracking ability and energy required to manipulate the regulator. The controller parameters that characterize the best candidates are sampling period, prediction horizon, and control horizon. The best alternatives are shown in Table 2.

Table 2: Optimal solutions according to reference tracking ability and energy requirements

Alternative (Cost)	*Sampling Period [s]*	*Prediction Horizon [samples]*	*Control Horizon [samples]*
1 (22101)	20	20	5
2 (22103)	20	40	10
3 (23846)	10	40	10
4 (23923)	10	20	5
5 (27307)	40	40	10

It is possible to state that alternatives 1 and 2 may be considered equally good in terms of reference tracking ability and energy requirements.

The quality of reference tracking also has to be evaluated and the computational time required for handling the neural network. The computational time needed for the simulation is a function of neural network complexity and reflects the cost of effort needed for the required accuracy by MPC. It is known that the MPC requires high quality of output prediction, and it is also known that the larger the neural network is, the accuracy is improved. This qualitative

parameter has been included in the evaluation to present the effect of neural network size and control system resolution on the accuracy and the cost of complexity. The controller parameters that characterize the best candidates are sampling period, prediction horizon, and control horizon. The best alternatives are shown in Table 3.

Table 3: Optimal solutions according to reference tracking ability and computational requirements

Alternative (Cost)	*Sampling Period [s]*	*Prediction Horizon [samples]*	*Control Horizon [samples]*
1 (22293)	20	20	5
2 (22982)	20	40	10
3 (25815)	10	40	10
4 (26898)	10	20	5
5 (27692)	40	40	10

The difference between alternative 1 and 2 has widened, and the best candidate became alternative 1.

The reference tracking ability and total error have significant value and may influence the results when considering the quality parameters in pairs. Therefore, the quality evaluation and the best candidate selection were also compared according to energy and computational requirements.

The controller parameters that characterize the best candidates are sampling period, prediction horizon, and control horizon. The best alternatives are shown in Table 4.

Table 4: Optimal solutions according to reference tracking ability and computational requirements

Alternative (Cost)	*Sampling Period [s]*	*Prediction Horizon [samples]*	*Control Horizon [samples]*
1 (310)	80	40	10
2 (465)	60	40	10
3 (614)	20	20	5
4 (719)	40	40	10
5 (778)	80	40	10

The difference between alternative 1 and 2 has widened, and the best candidate became alternative 1.

According to criteria shown in the previous sections, it is shown that although it is not the fastest alternative, the optimal structure of the MPC for the specific system – polypropylene reactor is the predictive model controller with a sampling period of the 20s, prediction horizon of 20 samples and control horizon of 5 samples.

The sampling period of the controller has a significant effect on the overall performance of the closed-loop response. The sampling period effect has been checked with a MPC configured with prediction horizon 40 samples and control horizon of 10 samples. The sampling period has been selected from the lowest interval of 5 seconds to the most extended interval of 80 seconds, without changing the controller configuration. The results are different for experiments with measurement noise applied to the feedback signals and situations without any noise. Figure 15 and Figure 16 display the effect of varying sampling periods on the qualitative parameters mentioned in the previous sections.

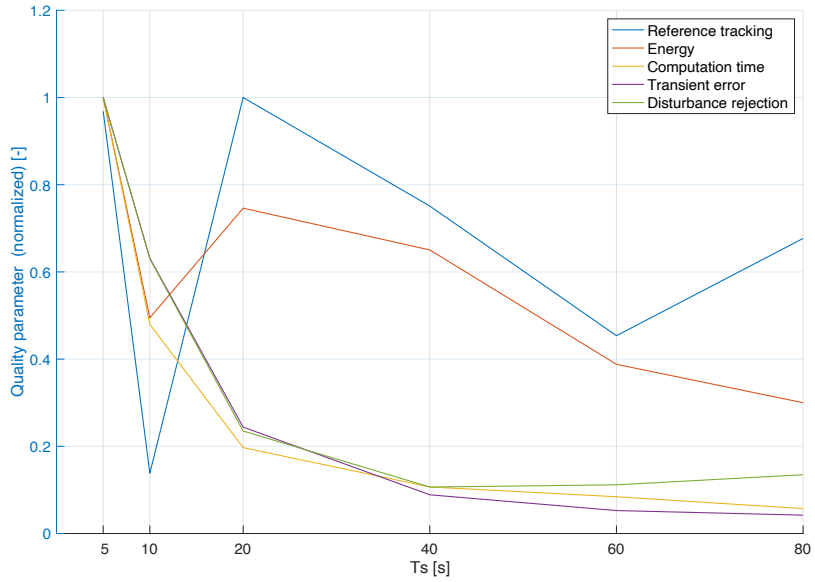

Figure 15: Sampling period effect on selected MPC configuration without noise

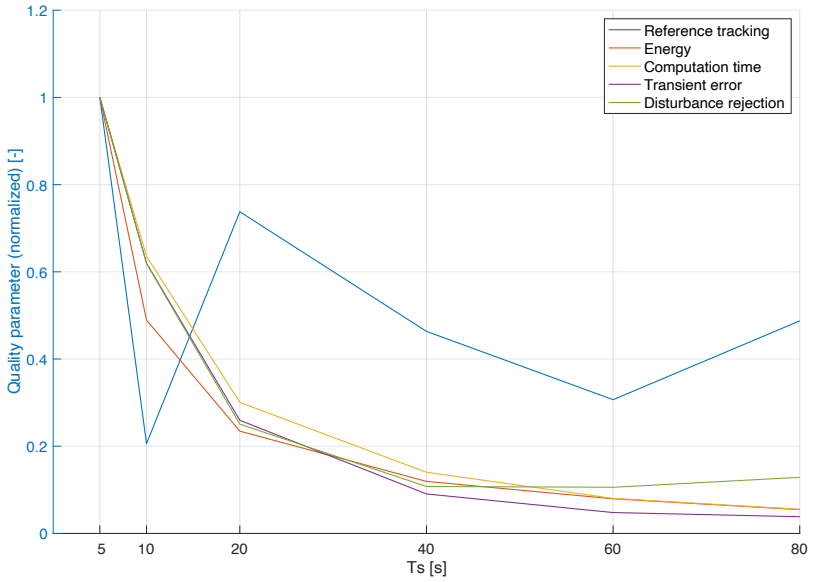

Figure 16: Sampling period effect on selected MPC configuration with random noise

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5. Achievements

The thesis provides a deep insight into the kinetic modeling of the specific chemical reaction. It is shown that the approach to the mathematical modeling of the kinetic process during the polymerization reaction is generally applicable in the control theory. The thesis proposes applying the kinetic model for MPC of a highly nonlinear process with discrete states. This thesis's hybrid process, with continuous nonlinear and discontinuous states, is based on the real plant. The simulations and experiments in environment Matlab have been conducted with real data captured at the existing plant with the plant operator's approval. The data have been recorded during one year of continuous operation of polypropylene unit.

The thesis proposes a solution to the control problem using a hybrid controller, which uses neural networks to predict and model the non-measurable states and presents a solution to the discrete states in a hybrid prediction model with discrete sub-model switching. Values and data used during the simulations have been compared to the real data and product production rates. The thesis also provides a deep analysis of the results and qualitative evaluation of different controller configurations.

Another achievement to be considered is the scalability and flexibility of the proposed control system. An analysis of the controller performance for multiple system configurations has been conducted again. The numerous neural networks' advantage compared to a single-network solution has been proven and analyzed using objective criteria.

Implementation of the ANN for feedback estimation can eliminate the current heuristic approach, which is highly dependent on the operator. Manual input of the process control can be reduced and thus increase the effectivity and safety.

The proposed approach provides a possibility for future development and extension with the control system's online adaptation according to expected or predicted operation mode. The process parameters and time delays does allow the online adaptation and training of the ANN estimator according to the actual catalyst properties. Further development of the proposed control strategy may bring a universal MPC with desired scalability and tunability of the online optimization. The proposed methodology with hybrid model can significantly improve the existing control strategies for wide spectrum of industrial processes.

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6. Publications

6.1. AFC International publications

AFC01 KARAS, Peter - KOZÁK, Štefan. Artificial neural network approach to modeling of polypropylene reactor. In *International Journal of Advances in Chemistry*. Vol. 3, No. 3/4 (2017), s. 1-14. ISSN 2455-7862.

AFC02 KARAS, Peter - KOZÁK, Štefan. Modeling and control of highly nonlinear complex process. In *2020 Cybernetics & Informatics (K&I) [electronic]: 30th International Conference. Velké Karlovice, Czech Republic. January 29-February 1, 2020*. 1. ed. Danvers: IEEE, 2020, [6] s. ISBN 978-1-7281-4381-1. In database: IEEE: 9039887; SCOPUS: 2-s2.0-85083117422; DOI: 10.1109/KI48306.2020.9039887.

6.2. AFD Local publications

AFD01 KARAS, Peter - KOZÁK, Štefan. Highly nonlinear process model using optimal artificial neural network. In 2018 Cybernetics & Informatics (K&I) [electronic]: 29th International Conference. Lazy pod Makytou, Slovakia. January 31-February 3, 2018. 1. Ed. Bratislava: Slovak Chemical Library, 2018, USB, [6] s. ISBN 978-1-5386-4420-1. In database: IEEE: 8337548; WOS: 000454633500019; SCOPUS: 2-s2.0-85050910195.

AFD02 KARAS, Peter - KOZÁK, Štefan. Nonlinear process prediction using neural network model. In ELITECH´19 [electronic]: 21st Conference of doctoral students. Bratislava, Slovakia. May 29, 2019. 1. ed. Bratislava: Spektrum STU, 2019, CD-ROM, [5] p. ISBN 978-80-227-4915-2.

AFD03 KARAS, Peter - KOZÁK, Štefan. Performance comparison of advanced and conventional control method of nonlinear chemical process. In ELITECH´20 [electronic]: 22nd Conference of doctoral students. Bratislava, Slovakia. May 27, 2020. 1. ed. Bratislava: Spektrum STU, 2020, [6] p. ISBN 978-80-227-5001-1.

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