Neural Network Based Softsensor for a Tubular Reactor

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Abstract

The paper deals with the mathematical modeling of a high pressure jacketed tubular reactor and the development of a neural network based softsensor for estimating the polymer quality at the exit of a tubular reactor. The reactor model consists of differential equations written as function of the dimensionless reactor length. The method of moments is used for describing the polymer molecular properties. The chain transfer to solvent process and the coolant flow are taken into account. The reactor mixture speed is assumed constant, the inlet pressure and the pulse valve effects are not included in the model. The paper develops the general concept of the softsensor and applies it to the problem of estimating the polymer quality. The softsensor is an artificial intelligence instrument and belongs to the class of inferential measurement techniques. The process variables not measurable are the initiator concentration and the heat transfer coefficient. The process information easily measurable and directly available for building the softsensor consists of the discrete temperature profile, the coolant flow temperature and the solvent concentration. As softsensor structure a feedforward neural neural network with one hidden layer is employed. The neural networks inputs consist of directly measurable process variables and process characteristics. The process characteristics (such as the area under the temperature profile peak, the peak location) compensate for the not measurable process variables. The solvent concentration proves to be an important input for the softsensor and improves significantly the softsensor approximation property.

Keywords: Mathematical modeling, Tubular reactor, Polymerization, Neural network, Softsensor.

1 Introduction

The paper investigates the possibility of building softsensors for the polymer quality (the weight average degree of polymerization) at the exit of a tubular reactor. This is extremely important because the measurement of polymer quality is needed for the control algorithm that regulates the end-use properties of the polymer. The practical applicability of a control methodology for a polymerization reactor, working well in simulations, is strongly influenced by the possibility of measuring precisely different process variables. The measurement of the weight average degree of polymerization is done with difficulty in practice (Zabisky *et al.*,

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1991; Nordhus *et al., 1997*) and basically three types of measurements are used (Joseph Schork *et al., 1993*): *inferential measurement, off-line tests* and *on-line measurement*. The inferential measurement uses a model relating some process variables or operating conditions (that can be changed during the normal functioning of the process) to the weight average degree of polymerization. Off-line tests can determine the polymer quality in the laboratory using techniques such as gel permeation chromatography. On-line measurements are performed by measuring the polymer melt index which is related to the weight average degree of polymerization. All these measuring methods are traditionally based on physical and chemical laws of the polymerization process. The general property of the reactors in the chemical industry is that they are highly nonlinear and important variables (such as the weight average degree of polymerization) can not be measured directly. The paper develops the general concept of the softsensor and applies it to the problem of estimating the weight average degree of polymerization. A lonely tubular reactor with a single injection of initiator/solvent with a preheater section and coolant flow is considered.

The paper is organized as follows: Section 2 shows the tubular reactor white model and its behavior. The formulation of the softsensor basic principle in the general case is presented in Section 3. Section 4 applies the softsensor basic principle to the tubular reactor for estimating the polymer quality; each step of the development of a neural network based softsensor is described. The conclusions are drawn in Section 5. In Appendix the numerical parameters and notations used in the text are given.

2   The tubular reactor white model

2.1   First principle model of the reactor

The present work deals with the chemical process of producing low density polyethylene (LDPE) in a high pressure polyethylene tubular reactor (Fig. 1). The tubular reactor is a circular tube, with certain diameter (d) and length (L), where the chemical reactions take place and polyethylene is produced.

A very simple description of the process is the following: the reactor feed (monomer + solvent) enters the reactor at certain temperature (T_o) and pressure, the initiator is injected to start up the chemical reactions, the reactor mixture is moving with a certain speed (v) inside the reactor and the polyethylene comes out (at temperature T_{out}) at the reactor end (the tubular reactor is the main part of the whole process flow of polyethylene; there are compressors, separators, product coolers, recycle systems (Zabisky *et al., 1991*) not presented here). The heat released during the chemical reactions is removed through the reactor jacket coolant flow (inlet temperature T_{ci}, outlet temperature T_{co}). The heat transfer coefficient (U) of the jacket and the coolant volumetric flow (F_w) are assumed constant along the reactor length. A common method for making polymers is **Free Radical Polymerization** and is thoroughly described (together with other methods: anionic, cationic and step-growth polymerization) in Joseph Schork *et al.* (1993). The monomer (raw material used to make polyethylene) consists of ethylene molecules (carbon-carbon double bonds). The polyethylene is a large molecule of repeating ethylene units. The main steps of *Free Radical Polymerization* are *initiation, propagation, termination and chain transfer reactions. Initiation*: the initiator breaks down into molecules called *free radicals*; these radicals have an unpaired electron who
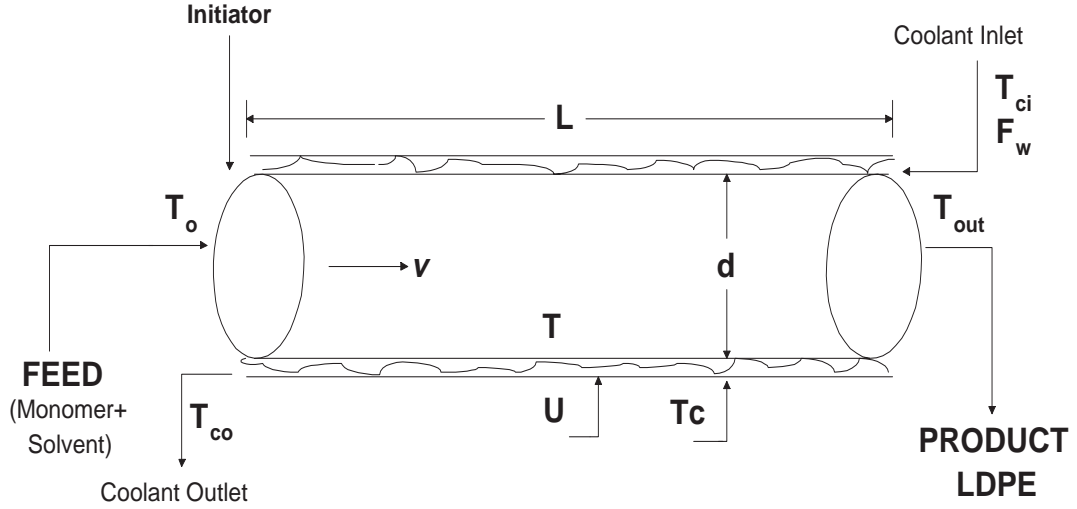
Figure 1: The polymerization tubular reactor diagram

will pair with another electron as soon as it has the opportunity. *Propagation*: the radicals, through the unpaired electron, will pair to the ethylene molecules forming *live* polyethylene chains; these live chains are growing by being concatenated with new ethylene molecules. *Termination*: the termination step ends the growing of the live polyethylene chains; it occurs either by *combination* (when two polyethylene live chains find each other, string together and stop growing), *chain transfer to polymer* (the unpaired electron at the end of a growing chain will pair with an electron from a carbon-hydrogen bond from another growing chain; the result is a *dead* polyethylene chain (does not grow anymore) and another live chain; the latter has carbons who have, instead of hydrogen, long chains of polyethylene attached to them; this is called *branched*, or *low density polyethylene*), *chain transfer to solvent* (the live chains stop growing by combining with the solvent molecules).

The tubular reactor model consisting of a set of highly nonlinear differential equations as function of the dimensionless reactor length is the following (the parameters are given in Appendix):

$$\frac{dC_i}{dz} = -\left(\frac{L}{v}\right)(K_d C_i) \tag{1}$$

$$\frac{dC_m}{dz} = -\left(\frac{L}{v}\right)(K_i C_R + K_p \lambda_0 + K_{tm}\lambda_0)C_m \tag{2}$$

$$\frac{dC_{si}}{dz} = -\left(\frac{L}{v}\right)(K_{tsi}\lambda_0 C_{si}) \tag{3}$$

$$\frac{dC_R}{dz} = \left(\frac{L}{v}\right)(2f_i K_d C_i - K_i C_R C_m) \tag{4}$$

$$\frac{d\lambda_0}{dz} = \left(\frac{L}{v}\right)(K_i C_R C_m - K_r \lambda_0^2) \tag{5}$$

$$\frac{d\lambda_1}{dz} = \left(\frac{L}{v}\right)[K_i C_R C_m + K_p \lambda_0 C_m - K_{tm} C_m(\lambda_1 - \lambda_0) + K_{tp}(\lambda_0 \mu_2 - \lambda_1 \mu_1) -$$
$$-K_r \lambda_0 \lambda_1 - K_{tsi} C_{si}(\lambda_1 - \lambda_0)] \tag{6}$$

$$\frac{d\mu_0}{dz} = \left(\frac{L}{v}\right)(K_{tm}\lambda_0 C_m + 0.5 K_r \lambda_0^2 + K_{tsi} C_{si} \lambda_0) \tag{7}$$

$$\frac{d(\lambda_1 + \mu_1)}{dz} \cong \frac{d\mu_1}{dz} = \left(\frac{L}{v}\right)(K_i C_R C_m + K_p \lambda_0 C_m + K_{tm}\lambda_0 C_m + K_{tsi} C_{si} \lambda_0) \tag{8}$$

$$\frac{d(\lambda_2 + \mu_2)}{dz} \cong \frac{d\mu_2}{dz} = \left(\frac{L}{v}\right)(K_{tm}\lambda_0 C_m + K_{tsi} C_{si} \lambda_0 + K_i C_R C_m + K_p \lambda_0 C_m +$$
$$+2K_p \lambda_1 C_m + K_r \lambda_1^2) \tag{9}$$

$$\frac{dT}{dz} = \left(\frac{1}{\rho C_p}\right)\left(\frac{L}{v}\right)\left[(-\Delta H_p)K_p C_m \lambda_0 - \frac{4U}{d}(T - T_c)K\right] \tag{10}$$

$$\frac{dT_c}{dz} = \frac{L \cdot \pi \cdot d \cdot U \cdot 4.1868 \cdot 10^{-3}}{F_w \cdot \rho_w \cdot Cp_w}(T_c - T) \tag{11}$$

$$X_{nr} = \frac{\lambda_1 + \mu_1}{\lambda_0 + \mu_0} \tag{12}$$

$$X_{wr} = \frac{\lambda_2 + \mu_2}{\lambda_1 + \mu_1} \approx \frac{\mu_2}{\lambda_1 + \mu_1} \tag{13}$$

The main references for building the reactor model is the work of Yoon (1982), Yoon and Rhee (1985) and Kiparissides *et al.* (1993). The model (Munoz, 1996; Anghelea, 1998) is written as function of the dimensionless reactor length and takes into account the chain transfer to solvent process and the coolant flow. The equations (1), (2), (3), (4) describe the variations of the initiator, monomer, solvent and radicals concentrations along the reactor length. The *live* (λ_0, λ_1) and *dead* (μ_0, μ_1, μ_2) leading moments (of the polymer chains distributions) variations are described by the equations (5)...(9). These leading moments are used for the calculation, according to (12) and (13), of the number and weight average degrees of polymerization (Kiparissides *et al.*, 1993). The variation of the temperature inside the reactor is described by equation (10) and of the coolant temperature (Anghelea, 1998) by equation (11). The parameters for the reaction rate constants (Arrhenius Equation: $K_x = K_{x0} e^{-\Delta E/(R_g T_{abs})}$) given in Yoon and Rhee (1985) are used. The chain transfer to solvent kinetic rate constant (K_{tsi}) parameters are $K_{x0} = 3.00 \cdot 10^7$ l/moles·sec and $\Delta E = 10000$ cal/moles. The reactor pressure is not included in the calculation of the kinetic rate constants. The coolant flow

equation (11) is written knowing that ρ_w=1 Kg/l; C_{pw}=4.18 KJ/Kg·°K; 1 cal=4.1868 Joules. The model is simulated using the parameters given in Yoon and Rhee (1985). The solvent concentration is considered 0 moles/l and the jacket temperature is assumed constant along the reactor length. The reactor performances (temperature profile, initiator and monomer conversion, number average degree of polymerization) are closely the same as in Yoon and Rhee (1985). Only one exception is encountered: the shape of the weight average degree of polymerization after the total consumption of initiator. Notice (Fig. 2) that the weight average degree of polymerization has an increasing shape close to the reactor end. For integrating the stiff differential system of equations a numerical differentiation procedure with backward differences is used. The parameters for the simulation in Fig. 2 are given in Appendix.
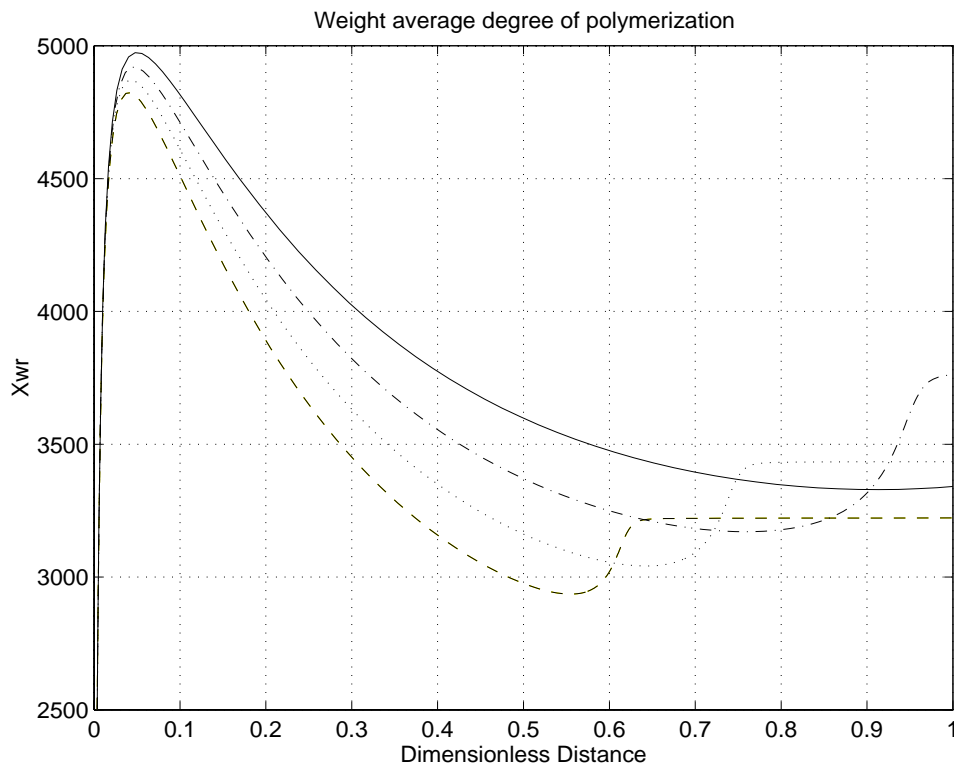

Figure 2: Profiles of weight average degree of polymerization (solid, dashdot, dotted, dashed) for various jacket temperatures (170,180,190,200)

2.2 White model behavior overview

The reactor with the jacket temperature constant and with the same parameters used by Yoon (1982) gives the same simulation results as reported in (Yoon, 1982; Yoon and Rhee, 1985) (with the exception in Fig. 2). For doing the simulations the heat transfer coefficient, feed conditions, jacket temperature and solvent concentration were varied. The complete list of simulation results is given in Anghelea (1998). The simulations performed lead to the following observations: when the jacket temperature increases the peak temperature increases and the peak location decreases; the exit monomer conversion increases but there exists a particular jacket temperature for which the exit monomer conversion reaches its maximum.

The exit weight average degree of polymerization varies when the jacket temperature varies. The heat transfer coefficient has a big influence on the reactor behavior; the temperature profiles along the reactor and other reactor performances change as the heat transfer coefficient varies. The peak temperature increases significantly and the peak location decreases as the initiator concentration increases. The change of the solvent concentration affects only the weight and number average degrees of polymerization, other reactor performances do not change. All these simulations were done for the reactor inlet temperature T_o=100 $^o C$. The same type of simulations were performed considering the reactor inlet temperature T_o=180 ^{o}C.

Typical temperature profiles along the reactor are presented in Fig. 3. As the jacket temperature increases the peak location decreases. The peak temperature increases significantly as the initiator concentration increases. Typical temperature profiles obtained taking into account the coolant equation are presented in Fig. 4. The coolant temperature profile decreases along the reactor. As the heat transfer coefficient increases, more heat is transferred through the jacket and the temperature in the reactor decreases. The parameters of the simulations in Fig. 3, 4 are given in Appendix.
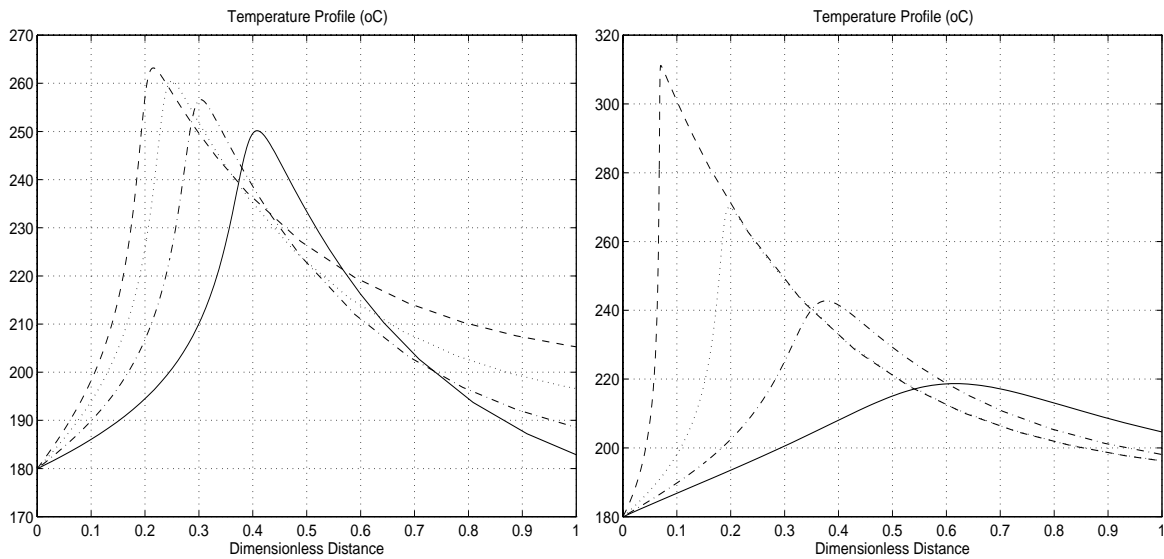

Figure 3: Temperature profiles (solid, dashdot, dotted, dashed) for different jacket temperatures (left) (170,180,190,200) and initiator concentrations (right) ($1 \cdot 10^{-4}$, $2.5 \cdot 10^{-4}$, $7.5 \cdot 10^{-4}$, $5.0 \cdot 10^{-3}$)

The solvent concentration influences only the average degrees of polymerization, other performances (monomer conversion, initiator conversion, temperature profile, cooling flow temperature profile) do not change. As a consequence using the solvent concentration as input for the softsensor improves significantly the estimation performances

3 The softsensor basic principle

A *softsensor* is a software program that uses artificial intelligence techniques to estimate process or quality variables difficult to measure in real time (due to the adverse process envi-
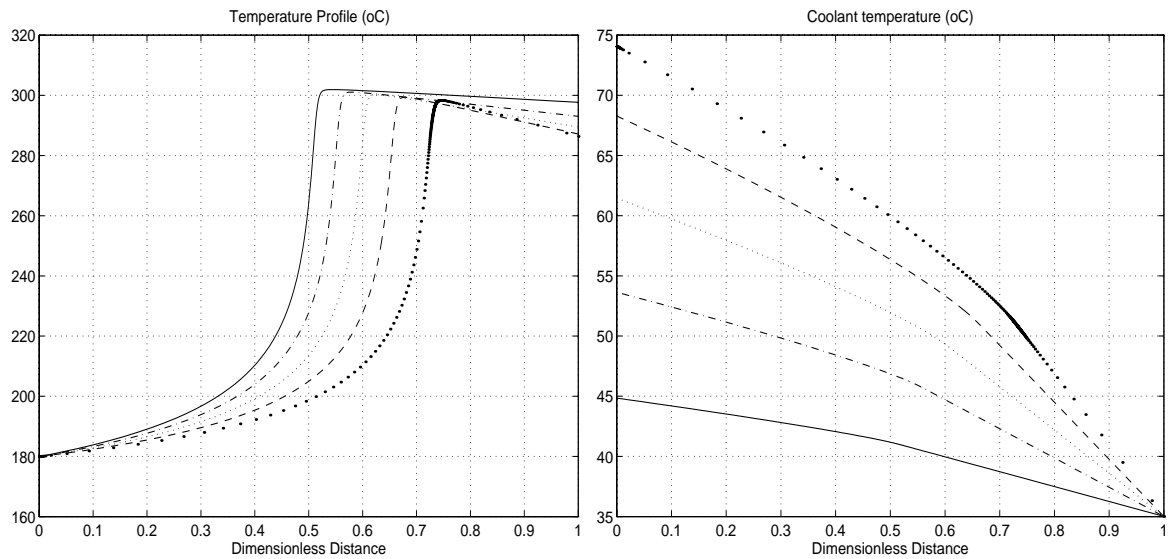
Figure 4: Temperature profiles (solid, dashdot, dotted, dashed, point) for different heat transfer coefficients (0.002,0.004,0.006,0.008,0.01)
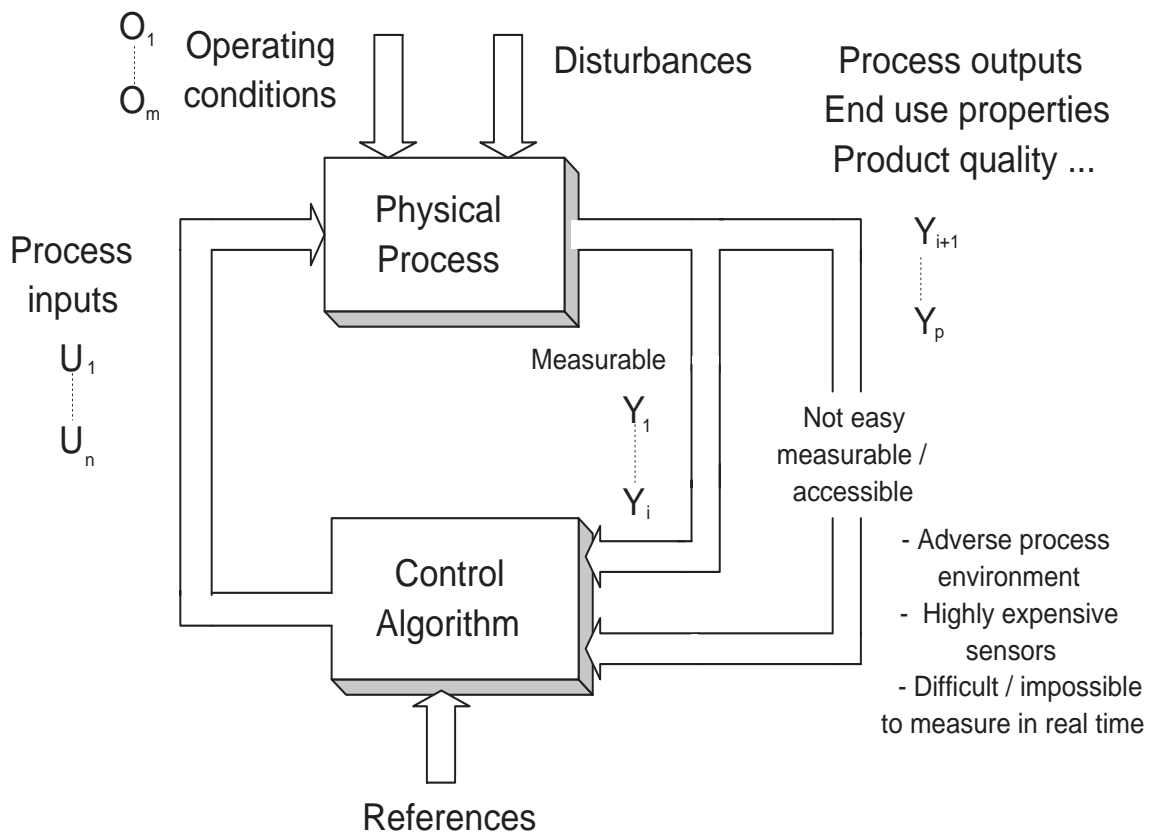

Figure 5: The typical process control loop

ronment, expensive sensors ...) (Anghelea, 1998). The typical process control loop (Anghelea, 1998) is suggested in Fig. 5. The available process information (assumed measurable) that can be used for building softsensors for $\mathbf{Y_{i+1}} \ldots \mathbf{Y_p}$ (process outputs, end-use properties, product quality indicators) consists of: the operating conditions $(\mathbf{O_1} \ldots \mathbf{O_m})$, the measurable process outputs $(\mathbf{Y_1} \ldots \mathbf{Y_i})$ and the process inputs $(\mathbf{U_1} \ldots \mathbf{U_n})$ (also the measurable disturbances, if there are any, can be taken into account). The softsensor (Fig. 6) uses the *easily measurable process information* for estimating the *difficult/not measurable* process or quality variables.

The *Inputs Selection Criterion/Method* block selects from the amount of information available the *relevant* and *useful* inputs for the softsensor $\mathbf{S_1} \ldots \mathbf{S_s}$. The outputs of the softsensor are the *estimations* $\mathbf{\hat{Y}_{i+1}} \ldots \mathbf{\hat{Y}_p}$ of the *real* outputs $\mathbf{Y_{i+1}} \ldots \mathbf{Y_p}$. The softsensor principle can be applied to processes characterized by excessive noise, severe nonlinearities or multivariable interactions.
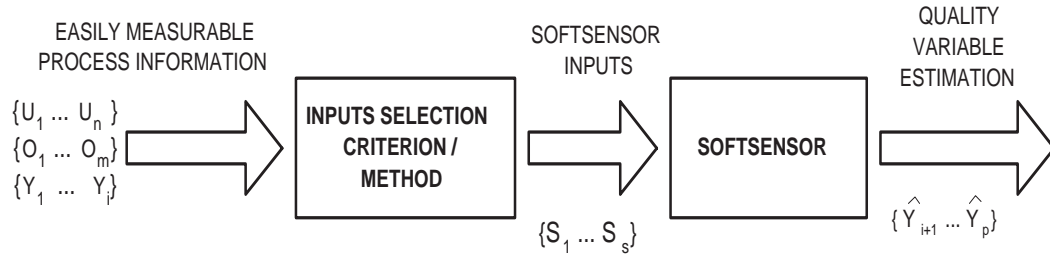

Figure 6: The softsensor basic principle

A problem which arises is to select from the amount of information available the *relevant and useful information* for the softsensor inputs (it makes no sense to use redundant or useless inputs). The inputs selection could be done by analyzing the process behavior and using the process experts experience. In this paper, for finding the softsensor inputs, a heuristic approach is used.

4 Softsensors for the polymer quality

4.1 The easily measurable process information

The available and measurable process information is the *temperature profile* $\mathbf{T}$ (in this study observed every *10 meters* along the reactor), the *solvent concentration* $(\mathbf{C_{si}})$ and the coolant inlet/outlet temperatures $(\mathbf{T_{ci}}, \mathbf{T_{co}})$. The reactor length is L=150 m and the reactor inlet temperature is T_o=180 ^0C. The area under the peak temperature $\mathbf{A_{pk}}$, the peak location $\mathbf{X_{pk}}$, the peak temperature $\mathbf{T_{pk}}$ and the total area under the temperature profile $\mathbf{A_{tot}}$ (Fig. 7) are used as inputs for the softsensor. All these quantities (equations (14),(15),(16),(17)) are calculated using the **discrete temperature profile** (consisting of the measurable temperatures $\mathbf{T_i}$, i=1 ... 15).
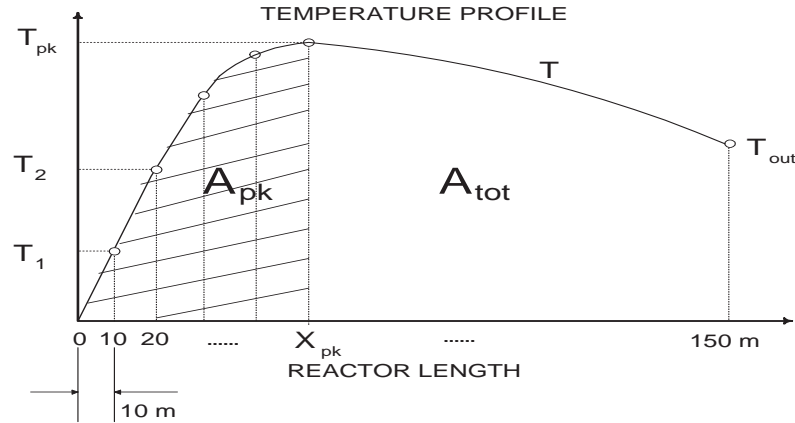
Figure 7: Definitions of temperature areas

$$T_{pk} = max\{T_i, \ \ i = 1...15\} \tag{14}$$

$$T(X_{pk}) = T_{pk} \tag{15}$$

$$A_{pk} = \int_0^{X_{pk}} T(x)dx, \ \ x \in \{10 \cdot i, \ i = 1...15\} \ \ (discrete \ \ integral) \tag{16}$$

$$A_{tot} = \int_0^{L} T(x)dx, \ \ x \in \{10 \cdot i, \ i = 1...15\} \ \ (discrete \ \ integral) \tag{17}$$

4.2   Looking for relevant information

In practice the weight average degree of polymerization ultimately affects the end-use properties of the polymer and it is not easy to measure. The difficulty is due to the deadtimes introduced (take a product sample, analyze it in the laboratory ...) and the methods used (gel permeation chromatography). In this section we look for any relationships that exist between the *inaccessible process information* and the *process characteristics* (as $\mathbf{A_{pk}}$, $\mathbf{A_{tot}}$).

Fig. 8 shows the areas under the temperature profile ($\mathbf{A_{pk}}$, $\mathbf{A_{tot}}$) as function of the initiator concentration for various heat transfer coefficients (the parameters of the simulation are given in Appendix). Notice that there are initiator concentrations for which there is a (bijective) relationship between the area under the peak and the heat transfer coefficient. Such relationships exist also between the total area under temperature profile and the heat transfer coefficient.

The areas ($\mathbf{A_{pk}}$, $\mathbf{A_{tot}}$) require calculations and temperature sensors placed along the reactor. If the temperature profile is approximated with *straight lines* then $\mathbf{A_{pk}}$ and $\mathbf{A_{tot}}$ depend on the product between the peak location with the peak temperature ($\mathbf{X_{pk} \cdot T_{pk}}$) and with the output reactor temperature ($\mathbf{X_{pk} \cdot T_{out}}$). Similar correspondences proved to exist between the initiator concentration, the heat transfer coefficient and $\mathbf{X_{pk} \cdot T_{pk}}$, $\mathbf{X_{pk} \cdot T_{out}}$. The idea is to compensate for the lack of the initiator concentration (this quantity is very
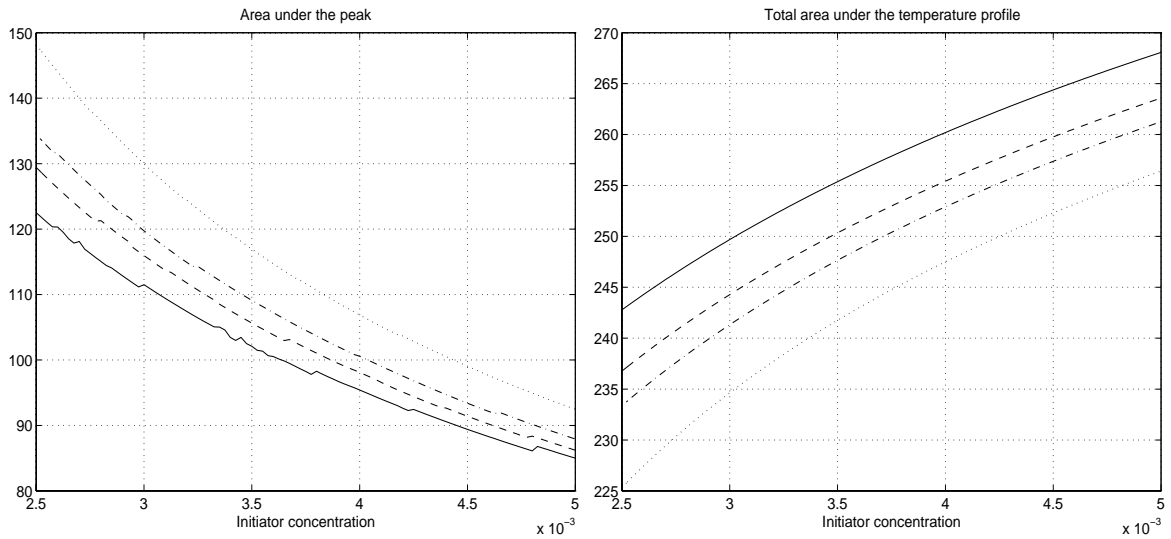
Figure 8: Areas (solid, dashed, dashdot, dotted) under the temperature profiles as function of the initiator concentration for various heat transfer coefficients (0.002,0.004,0.005,0.007)

small and is a combination of different chemical substances) and the heat transfer coefficient (the reactor mixture while it is moving to the reactor end is sticking on the reactor wall and makes the measurement of the heat transfer coefficient difficult).

The goal is to use the information in the temperature profile for estimating the weight average degree of polymerization. The reason is that the temperature profile is the *deterministic outcome* of the chemical reactions taking place in the reactor as the *consequence* of certain process variables and operating conditions. The process variables not measurable can be inferred, due to the *deterministic aspect*, from the temperature profile or other measurable process information.

4.3 Neural network based softsensors for the polymer quality

The artificial neural networks consist of a number of simple processing elements or units called neurons. The neurons are interconnected, exchange information and implement distributed processing. One of the most important properties of the neural networks is that they satisfy the *Universal Approximation Property* (Hunt *et al.,* 1995): *they are able to approximate an arbitrary continuous function defined on a compact set to an arbitrary degree of accuracy.*

Important elements of the artificial neural networks are the model structure (regressor vector) selection and the neural network training. The model structure selection is concerned with the selection of the number of hidden layers and the number of neurons (and activation functions) for each layer. During the training process the neural network's parameters (neurons biases and weights) are continuously adjusted for realizing the input-output dependence with the desired accuracy. For detailed explanations about neural networks structure, training and validation methods and other aspects of the neural networks see Warwick *et al.* (1992), Haykin (1994), Hunt *et al.* (1995).

As softsensor structure the feedforward neural network (Haykin, 1994) with one hidden layer is employed. The neural network is trained using Levenberg-Marquardt (Declercq and De Keyser, 1995) minimization algorithm (this algorithm ensures a relatively fast convergence and robustness against local minima). A lot of simulations and experiments were done for choosing the type of activation function and the number of neurons in the hidden layer. For this purpose the neural networks were trained for a number of epochs and the activation function was chosen by looking at SSE (Sum Squared network Error) (Haykin, 1994) and MGE (Mean Global Error) (Anghelea, 1998) over both training and validation sets. The mean global error definition for N training (validation) points is:

$$MGE = \sum_{i=1}^{N} \frac{|WM_i - NN_i|}{WM_i} \tag{18}$$

where WM_i is the exit weight average degree of polymerization calculated using the white model and NN_i is the exit weight average degree of polymerization calculated using the neural network.
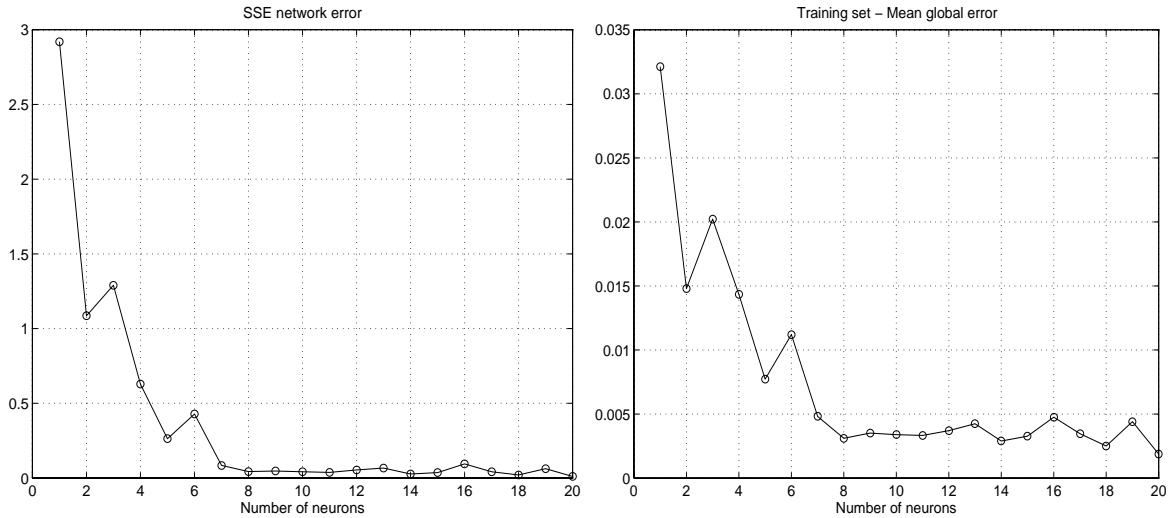

Figure 9: Choosing the number of neurons in the hidden layer

The neural networks inputs were scaled in the interval [-1 1] and the outputs in the interval [1 2]. Typical graphs obtained for every neural network are shown in Fig. 9. The SSE and MGE over the training set are represented as function of the number of neurons in the hidden layer (in this case the number of neurons should be greater than 8). The activation function of the neurons in the hidden layer was chosen by looking at the same indicators (SSE, MGE). For all neural networks presented in the following the hidden layer neurons have log-sigmoid (Haykin, 1994) activation functions.

The reactor length is L=150 m and the reactor inlet temperature T_o=180 ^oC. The parameters varied for data generation are the initiator concentration, the solvent concentration, the heat transfer coefficient and the coolant outlet temperature. The coolant volumetric flow

PARAMETER	RANGE
Initiator concentration, C_i	$[2.5 \cdot 10^{-3} \ldots \ 5 \cdot 10^{-3}]$ moles/l
Solvent concentration, C_{si}	$[0 \ldots 0.05]$ moles/l
Heat transfer coefficient, U	$[0.002 \ldots 0.007]$ cal/$cm^2 \cdot$sec$\cdot$°C
Coolant outlet temperature, T_{co}	$[65 \ldots 70]$ °C

Table 1: Parameter ranges for data generation

is considered constant $F_w = 10$ l/sec. The ranges for the parameters are given in Table 1.
In order to generate the training/validation sets, for each parameter 6 equidistant values were selected; this leads to 1296 points for each training and validation set. The neural networks inputs are summarized in Table 2 and their performances in Table 3 (MPET denotes the maximum percentage error over the training set, MPEV denotes the maximum percentage error over the validation set).

NNET NR.	INPUTS	OUTPUT
1.	$T_{pk}, T_{co}, T_{out}, T_{ci}, X_{pk}, C_{si}$	Exit X_{wr}
2.	$T_{pk}, T_{co}, T_{out}, T_{ci}, A_{pk}, A_{tot}, X_{pk}$	Exit X_{wr}
3.	$T_{pk}, T_{co}, T_{out}, T_{ci}, A_{pk}, A_{tot}, X_{pk}, C_{si}$	Exit X_{wr}
4.	$T_{pk}, T_{co}, T_{out}, T_{ci}, X_{pk} \cdot T_{pk}, X_{pk} \cdot T_{out}, X_{pk}, C_{si}$	Exit X_{wr}
5.	$T_1, T_2, T_3, T_4, T_5, T_6, T_7, T_8, T_9, T_{10}, T_{11}, T_{12}, T_{13}, T_{14}, T_{15}$	Exit X_{wr}
6.	$T_1, T_2, T_3, T_4, T_5, T_6, T_7, T_8, T_9, T_{10}, T_{11}, T_{12}, T_{13}, T_{14}, T_{15}, C_{si}$	Exit X_{wr}

Table 2: Neural networks inputs

NNET NR.	Hidden neurons	Training epochs	MPET	MPEV
1.	8	80	0.102 %	0.310 %
2.	8	60	18.01 %	14.86 %
3.	8	75	0.091 %	0.054 %
4.	10	50	0.51 %	0.56 %
5.	15	50	22.50 %	22.13 %
6.	12	50	0.098 %	0.152 %

Table 3: Neural networks performances

The best performances are obtained by the third neural network (Table 2). The process information needed for the neural network inputs consists of the discrete reactor temperature profile, the cooling flow inlet/outlet temperatures and the solvent concentration. The approximation capability of this neural network (softsensor) over the training/validation sets is presented in Fig. 10.

5   Conclusions

A mathematical model of the high pressure tubular reactor for producing low density polyethylene is developed. The model is based on the equations of *Yoon and Kiparissides*, takes into account the chain transfer to solvent process and includes the coolant flow. The white model
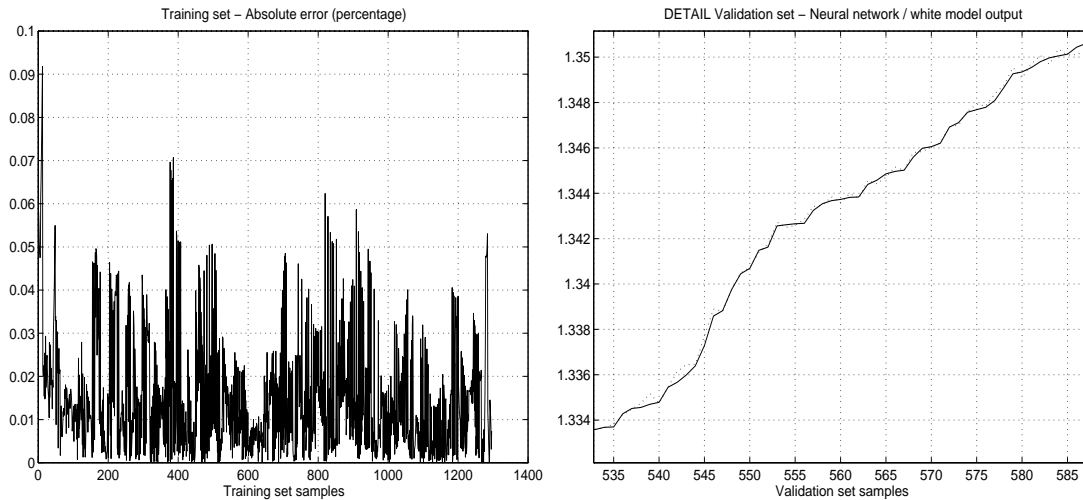
Figure 10: Softsensor performances

simulations are compared with the results obtained by *Yoon*. Similar simulation results are obtained except the shape of the weight average degree of polymerization after the total initiator consumption. The practical expertise and assistance was used for developing the model.

The softsensor basic principle is developed and applied for estimating the polymer quality (weight average degree of polymerization) at the exit of the tubular reactor (with preheater section and one feed/initiator injection). A study is done for finding the relevant information consisting of areas (under the peak temperature, under the total temperature profile) or other process characteristics (peak location) for compensating the unmeasurable process variables. The softsensors consist of feedforward neural networks with one hidden layer (log-sigmoid activation functions for the neurons in the hidden layer). Because real-life process data is not available for the present study we generate data using the white model by varying the initial conditions. The generated data is used afterwards for training/validating the neural networks. The parameters varied for generating the data are the initiator concentration, the solvent concentration, the heat transfer coefficient and the coolant outlet temperature.

The temperature profile only is insufficient for estimating the exit weight average degree of polymerization. Big estimation errors are obtained by a neural network having as inputs only temperatures along the reactor. The solvent concentration proves to be an important input for the softsensor and improves significantly the performances. The best performances are obtained by a neural network having as inputs: the peak temperature, the peak location, the area under the peak, the total area under the temperature profile, the solvent concentration, the outlet reactor temperature and the coolant inlet/outlet temperatures.

Appendix

PARAMETERS FOR THE REACTOR MODEL: C_i (moles/l)-Concentration for the initiator; C_{si} (moles/l)-Concentration for the solvent; C_m (moles/l)-Concentration for the monomer; C_R(moles/l)-Concentration for the radicals; K_d (1/sec)-Rate constant for dissociation of ini-

tiator; K_{tsi} (1/moles·sec)-Rate constant for chain transfer to solvent; K_{tm} (1/moles·sec)-Rate constant for chain transfer to monomer; K_{tp} (1/moles·sec)-Rate constant for chain transfer to polymer; K_r (1/moles·sec)-Rate constant for termination by combination; K_i (1/moles·sec)-Radicals rate constant; K_p (1/moles·sec)-Propagation rate constant; v (cm/sec)-Reaction mixture velocity; d (cm)-Inside tube diameter; F_w (l/sec)-Coolant volumetric flow; ρ_w (Kg/l)-Water density; C_{pw} (KJ/Kg·°K)-Water specific heat capacity; f_i-Initiator efficiency; L (cm)-Reactor length; z-Dimensionless axial distance; ρ (g/cm^3)-Reaction mixture density; C_p (cal/g·°C)-Specific heat capacity; T (°C)-Reaction temperature; T_c (°C)-Jacket temperature; T_o (°C)-Reaction inlet temperature; $-\Delta H_p$ (cal/moles)-Heat of polymerization reaction; U $(cal/cm^2·sec·°C)$-Heat transfer coefficient; ΔE (cal/moles)-Activation energy; R_g (cal/mol·°K)-Universal gas constant; λ_n (moles/l)-nth moment with respect to the NCLD (Number Chain Length Distribution) of "live" polymer; μ_n (moles/l)-nth moment with respect to the NCLD of "dead" polymer; K (cm^3/l)-Scaling factor (for unit conversion); x (cm)-Axial distance; X_{nr}-Number average degree of polymerization; X_{wr}-Weight average degree of polymerization.

KINETIC RATE CONSTANTS (K_x, K_{x0}, ΔE) (Arrhenius Equation: $K_x = K_{x0} e^{-\Delta E/(R_g T_{abs})}$): K_d, $1.60 \cdot 10^{16}$ sec^{-1}, 38400 cal/moles; K_i, $2.95 \cdot 10^7$ l/moles·sec, 7091 cal/moles; K_p, $2.95 \cdot 10^7$ l/moles·sec, 7091 cal/moles; K_{tm}, $5.83 \cdot 10^5$ l/moles·sec, 10090 cal/moles; K_{tp}, $9.00 \cdot 10^5$ l/moles·sec, 9000 cal/moles; K_r, $1.60 \cdot 10^9$ l/moles·sec, 2400 cal/moles; K_{tsi}, $3.00 \cdot 10^7$ l/moles·sec, 10000 cal/moles.

CONSTANT SYSTEM PARAMETERS: $-\Delta H_p$=22000 cal/moles; f_i=0.5; d=5 cm; K=10^3; ρC_p=600 g/cm^3; R_g=1.987 cal/moles·°K; v=10 m/sec.

STANDARD SYSTEM PARAMETERS: C_m=18 moles/l; C_i=$5 \cdot 10^{-4}$ moles/l; T_o=100 °C; T_c=190 °C; U=0.03 $cal/cm^2·sec·°C$.

SIMULATION PARAMETERS: The simulations use the constant/standard system parameters presented above; for each simulation only the parameters with other values are given. *Simulation in Fig. 2*: L=800 m, C_{si}=0 moles/l; for different jacket temperatures T_c=170, 180, 190, 200 °C. *Simulation in Fig. 3 left side*: T_o=180 °C, L=400 m, C_{si}=0 moles/l; for different jacket temperatures T_c=170, 180, 190, 200 °C. *Simulation in Fig. 3 right side*: T_o=180 °C, L=400 m, C_{si}=0.01 moles/l; for different initiator concentrations C_i=$1 \cdot 10^{-4}$,$2.5 \cdot 10^{-4}$, $7.5 \cdot 10^{-4}$,$5.0 \cdot 10^{-3}$ moles/l. *Simulation in Fig. 4*: L=150 m, T_o=180 °C, C_{si}=0 moles/l, C_i=$3 \cdot 10^{-3}$ moles/l, T_{ci}=35 °C, F_w=10 l/sec; for different heat transfer coefficients U=0.002, 0.004, 0.006, 0.008, 0.01 $cal/cm^2·sec·°C$.

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