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Development of Black-box Models for Industrial-scale Steam Crackers

MASTER'S THESIS

to achieve the university degree of

Diplom-Ingenieur

Master's degree programme: Chemical and Process Engineering
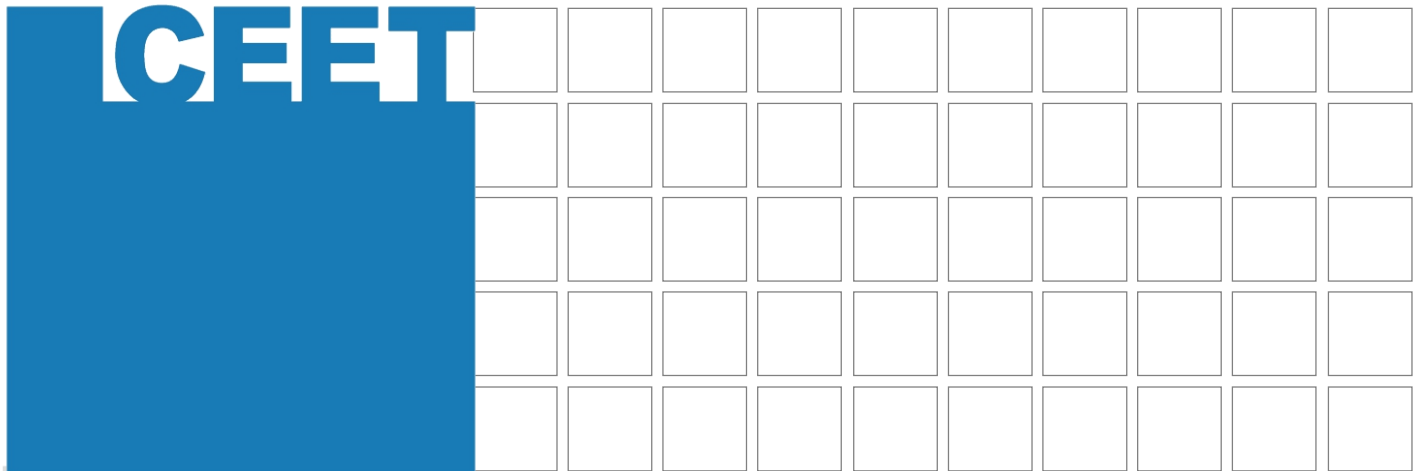
submitted to

Graz University of Technology

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Institute of Chemical Engineering and Environmental Technology

Graz, April 2018

Technische Universität Graz
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Master's Thesis

by

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Task description

Steam Cracking is the most common process for ethylene and propylene production. The process consists of (1) steam cracker furnaces and (2) the downstream-processing part. When it comes to process simulation of the whole plant, these two parts are modeled by two considerably different simulation approaches. While downstream-processing is usually modeled using a commercial simulation tool like KBC Petro-Sim, the state-of-the-art method for simulation of the radiant section of steam crackers is a kinetic radical model, considering more than 100 product components. These kinetic simulations are very accurate but expensive in terms of CPU time, in particular when it comes to refinery-wide optimizations. Therefore, this work aims at developing a fast-computing black-box model of the reactor effluent composition for different feed-stocks, reactor geometries and other process parameters, based on simulation data from rigorous kinetic simulations. For the black-box-model, the suitability of different approaches like polynomials and neural networks is investigated.

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Kurzfassung

Steam-Cracken ist der meist verwendete Prozess zur Herstellung von leichten Olefinen, wie Ethylen, Propylen und Butadien. Die Reaktionen in den Spaltöfen werden heutzutage mit einem Radikal-Kinetik-Simulationsprogramm berechnet, welches durch die Kinetik in seiner Geschwindigkeit stark eingeschränkt ist. Damit ist diese Methode zur Berechnung der Spaltgas-Zusammensetzung für raffinerieweite Optimierungen zumeist ungeeignet. In dieser Arbeit werden zwei verschiedene Arten von Black-Box-Modellen für 6 unterschiedliche Reaktortypen und variierende Betriebsweisen entwickelt. Als erster Ansatz kommen neuronale Netze, als zweiter das klassische Fitten von Polynomen als Black-Box-Modell für die Spaltgaszusammensetzung zum Einsatz. Ein Vergleich mit Validierungsdaten zeigt, dass neuronale Netze für flüssige Spaltofen-Einsätze sehr gut geeignet sind, während sie für gasförmige Einsätze größere Abweichungen aufweisen. Die Modelle auf Polynom-Basis zeigen erwartungsgemäß größere Abweichungen, sind aber für vereinfachte Berechnungen brauchbar.

Abstract

Steam cracking is the most common process for production of light olefins, such as ethylene, propylene and butadiene. The state-of-the-art method for simulation of the radiant section of steam crackers is the use of radical kinetic models, thereby requiring large amounts of computational effort. For this reason, this approach is generally limited for running plant-wide optimizations. Therefore, this work aims at developing a fast-computing black-box model of the reactor effluent composition for different feedstocks, reactor geometries and other process parameters, based on simulation data from rigorous kinetic simulations. Two modeling approaches are investigated: training of neural networks and classical fitting of polynomials. Six different reactor types are modeled using both approaches. The data basis is generated by simulations with radical kinetic software. As a result, the neural networks show a good prediction performance for liquid feedstocks, while the models for processing gaseous feedstocks show larger deviations to validation data. The simple polynomial approach performs not that good, but is suitable for simplified calculations.

Contents

1   Introduction

Light olefins are considered to be one of the most important feedstocks in the petro-chemical industry. The main part of them is used for plastic material production, especially ethylene and propylene are processed in large amounts. The demand for them is still increasing, arising from economic growth. [1, p. 171]

The technology utilized for the production of these light olefins is steam cracking, where hydrocarbons are thermally cracked in the presence of steam. This technology is proven and has an excessive energy consumption, due to the fact, that the cracking process takes place at temperatures up to 900°C and the heat has to be provided by gas burners. Even though the greenhouse gas emissions of this process are high, it is the only available technology to cover the large demands of olefins for the petro-chemical industry. [2, pp. 102-105]

Steam cracking produces a wide range of hydrocarbons, where hydrogen, ethylene, propylene and 1,3-butadiene represent the high-value-chemicals, most of the by-products are also quite valuable.
The cracking process takes place in cracking-furnaces, where the hydrocarbon and steam feed is heated and thereby cracked in so-called cracking-coils. At the outlet of the coils the gas is immediately quenched. Therefore, this cracking process determines the product-mix leaving the highly complex downstream-processing. Due to the fact that steam cracking is highly sensitive to the cracking temperature, residence time and feedstock-selection, ranging from ethane over LPG to gasoline and gasoil, the prediction of the reaction products is a challenging task. [2, pp. 105-107]

The state-of-the-art commercial simulation tool for these purposes utilizes a radical-kinetic reaction scheme in a 1-D reactor simulation. This simulation method provides a high grade of flexibility and precision on one hand, but, on the other hand, requires large amounts of CPU time for the simulation, which can be a bottleneck when it comes to site-wide simulations.

This work aims at finding an answer to the discrepancy of high prediction precision and computation time, using the exemplary of a real-life ethylene plant, running 10 steam cracking furnaces.

The modelling approach utilizes a large amount of radical kinetic simulations as data basis for (1) statistical regression and (2) training of feed-forward neural-networks to develop a model of the reactor-effluent composition. The reason for the selection of simulation data instead of measurement data is the narrow operating window of the existing plant, which does not have the necessary variety for the desired wide-range-models.

For each reactor geometry its possible feedstock combinations and operation conditions are determined and simulated with a radical kinetic simulation tool. From this simulation data, the reactor effluent compositions are extracted and processed with Wolfram Mathematica. A polynomial-fit model is attempted and furthermore feed-forward neural networks are designed and trained.

Finally, these two modelling approaches are compared to simulation results and measured data from the plant.

2 Process and mathematical basics

This chapter is aimed to explain the basics and key issues in steam cracking, the wide field of neural networks and statistics utilized for this work.

2.1 Ethylene plant

2.1.1 Overview

Modern ethylene plants are very large and highly integrated systems, where the cracking furnace section produces the cracked gas, which gets fractionated in the following downstream processing section. Process temperatures reach from 700 to 900°C at the cracking coil outlets to about -170°C for hydrogen separation, resulting in an excessive energy consumption, even though many efforts are invested in highly cross-linked energy recovery systems. In figure 2-1 a compressed flow chart of a typical ethylene plant is shown. [2, pp. 102-103]

Furnace Section
- Feed management
- Cracking furnaces
- Energy recovery – HPS production

Quench Section
- Fuel oil separation
- PyGas separation

Compression Section
- PyGas separation
- LPG separation

Distillation Section
- Ethane/ethylene splitting
- Propane/propylene splitting
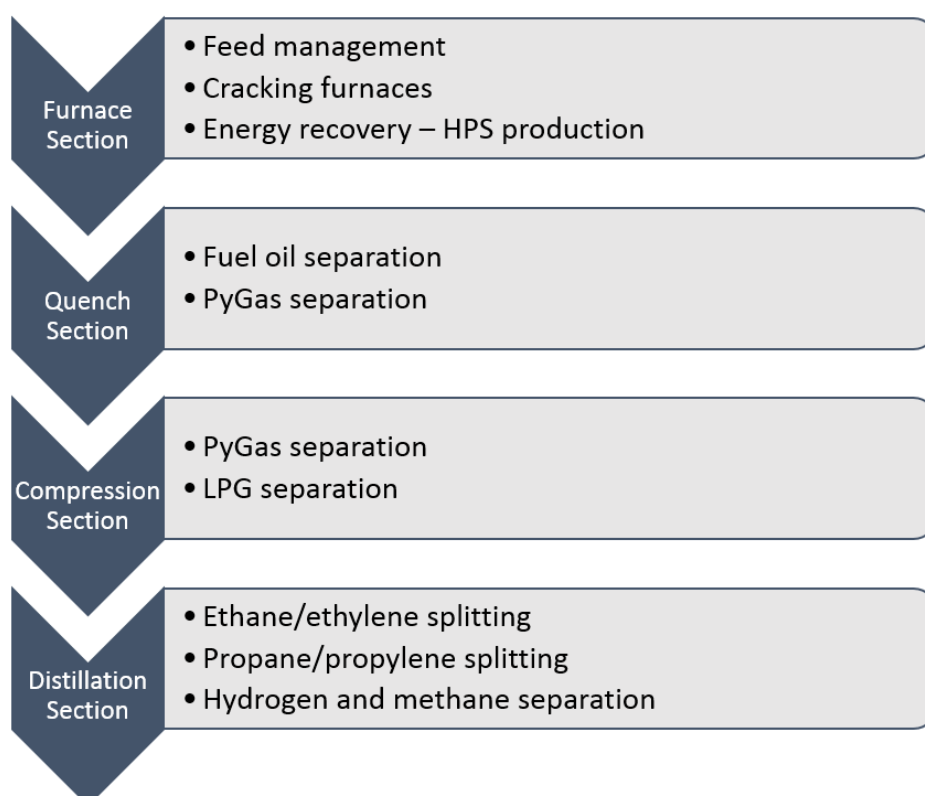- Hydrogen and methane separation

Figure 2-1: ethylene plant - flow chart

The furnace section also contains the feed management, controlling and selecting the feed mass flows to the cracking. Typically, a mix of liquid and gaseous feed types

is used and often mixed for so-called co-cracking. A more detailed description of the cracking furnaces and its energy recovery systems can be found in 2.1.3.4.

The quenching section's task is to cool the cracked gas further down, separating fuel oil and pyrolysis gas by washing the gas with fuel oil and water.

By compressing the gas in multiple stages, further liquids can be separated, in particular, pyrolysis gas at the beginning and C4-fractions at the end of the compression line. Due to the high throughputs this compression line is commonly powered by high pressure steam (HPS) and shows a high energy consumption.

The last section, consisting of many distillation columns, splits the remaining gas into its components. Typically, hydrogen, methane, ethane, ethylene, propane and propylene are separated with a very high purity, depending on internal and external demands.

2.1.2   Feeds and products

Modern ethylene plants are built to handle many different feed types, often defined by the refinery driving the respective ethylene plant or a nearby refinery providing the feedstocks to the cracking furnaces. The feedstocks vary by the global location of the plants, North American plants generally utilize large amounts of ethane, driven by the fracking boom, while European plants mainly use liquid feedstocks. [2, p. 103]

The feed types utilized by the considered ethylene plant are ethane, propane, C4-mixtures as well as different naphtha fractions up to fuel oil. Normally, ethane and C3/C4 mixtures are cracked separately. By mixing C3/C4 fractions with naphthas the so-called co-cracking is realized.

The considered ethylene plant as a part of a refinery is supplied with many different feed streams. With its flexibility in feed selection, it provides more flexibility to the refinery without utilizing too much storage capacity. The ethylene plant runs 10 steam cracking furnaces, some of them are realized as the same types in parallel.

Table 2-1 gives an overview of the feed types which can be processed by the particular furnaces.

It can be seen, that 3 furnaces are processing only liquid feeds, while 2 furnaces are only processing gaseous feed types. The others are processing liquid feeds as well as all kinds of gaseous feeds in co-cracking operation mode. Typically, the coil outlet temperatures are in a range of 780 to 860°C for liquid feeds, while gaseous feeds are preferably cracked at the higher end of this range.

Table 2-1: ethylene plant - feed selection

Feed type	Furnace									
	1	2	3	3	5	6	7	8	9	10
Naphta 1									x	x
Naphta 2	x	x	x	x	x	x	x			
Naphta 3	x	x	x	x	x	x	x			
Naphta 4	x									
Ethane		x	x	x	x	x	x	x	x	
Propane		x	x	x	x	x	x	x		
C4-Mixes		x	x	x	x	x	x			

The separation section of an ethylene plant offers a broad product mix, typical examples of those chemicals are listed in table 2-2.

Table 2-2: ethylene plant - products

Hydrogen	Propylene	Light Pyrolysis Gas
Methane	Propane	Heavy Pyrolysis Gas
Ethylene	Butadiene	Benzene
Ethane	C4-Mixes (LPG)	Fuel Oil

Due to its great cracking yields ethane and propane are recycled as furnace feed, also the C4-fraction is often fed to the furnaces.

2.1.3   Steam cracking

Steam cracking is a highly endothermic process where hydrocarbons, mixed with dilution steam, are decomposed thermally. The reactions take place in plug flow reactors, which are realized as cracking coils hanging in a firebox. Detailed information about cracking furnaces can be found in section 2.1.3.

The mix of hydrocarbons and steam is fed to the cracking coils with a temperature of about 500 to 620°C and leaves the reactor with about 700 to 900°C, where it is transferred to the so-called transferline exchangers, which quench the reaction, resulting in a temperature-level of about 400°C.

The reaction products mainly consist of light gases, mostly hydrogen, methane, ethane, propane, ethylene and propylene, but also an appreciable amount of C4-paraffins and olefins is produced. The rest of the reactor effluent consists of all possible hydrocarbons ranging to heavy gas oil and pyrolysis residues. The product mix can be shifted by varying several reactor parameters, and therefore they must be controlled and optimized to meet the external product demands of the plant. [2, p. 106]

In the following, these main parameters are listed.

2.1.3.1   Reactor temperature

The reactor temperature is measured on the reactor exit and must be controlled by the firing duty of the burners. Due to the endothermic reactions this parameter has a high impact to the reactor product mix. In table 2-3 the main reactions occurring are listed. [2, p. 106]

Table 2-3: main reactions in steam cracking [3, p. 3403]

reaction type	activation energy [kJ/mol]
H-abstraction – formation of a primary radical	50
H-abstraction – formation of a secondary radical	40
H-abstraction – formation of a tertiary radical	30
C-C – bond breaking	120
C-H – bond breaking	170
addition	20
isomerization	50

Due to the high activation energies of the C-C and C-H – breaking reactions, those are preferably taking place at high temperatures, whereas low temperatures lead to larger molecules by addition and other recombination reactions.

The effect of the so-called coil-outlet-temperature (COT) to the reactor products is demonstrated in figure 2-2, where a naphta feed is cracked at typical conditions.
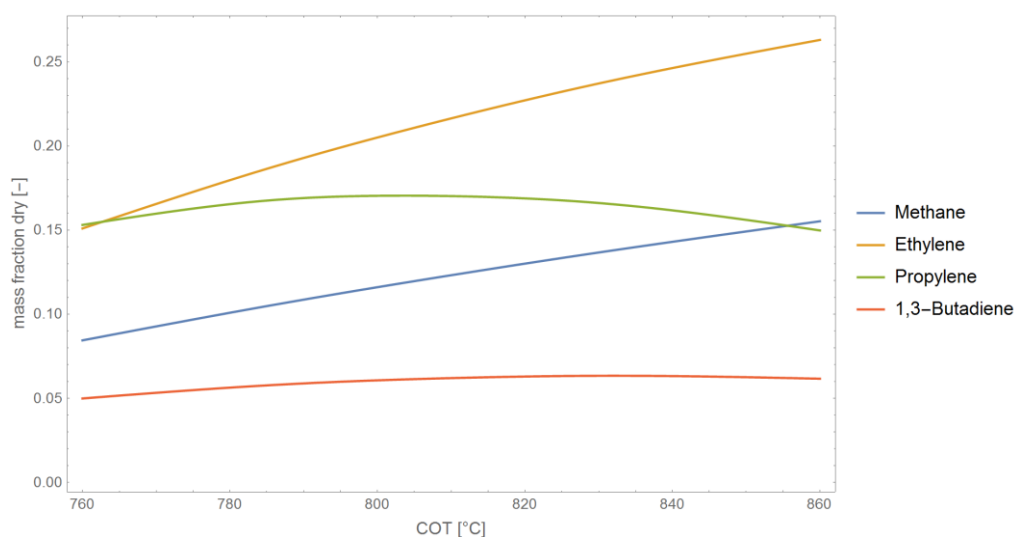

Figure 2-2: temperature dependency of reactor products

A high COT results in a high ethylene mass fraction, while the propylene mass fraction shows a maximum at lower temperatures. This shows how the product mix can

be influenced by varying the COT. It has to be pointed out, that a high COT causes a higher coking rate, therefore resulting in a lower reactor run length. [2, p. 106]

2.1.3.2   Residence time

The residence time has to be chosen in a way that the hydrocarbons have enough time to decompose on one hand, but, on the other hand, must be limited to prevent the intermediate reaction products from condensing reactions. It is controlled by the reactor geometry and the reactor feed rate. Modern steam cracking furnaces are designed for residence times between 0.08s and 0.3s. [2, p. 107]

2.1.3.3   Dilution steam

The reactor feed is premixed with the hydrocarbon feed before entering the cracking section of the furnace. The amount of dilution steam addition is calculated on weight basis, typically in a range of 0.3 to 0.7 kg steam/kg hydrocarbon, depending on the chosen feed type. It functions as an inert inside the reactor, reducing the fugacity of the hydrocarbons and thereby reducing the coking rate of the cracking coils. [2, p. 106]

The residence time is therefore highly affected by this parameter, due to the fact that dilution steam is also fed to the reactor.

2.1.3.4   Steam cracking furnace

The cracking furnace can be divided into a radiant section, where the cracking reactions occur, and into a convection section, containing large heat transfer surfaces for energy recovery and steam production. Typically, a cracking furnace is built up of 2 or more fireboxes, containing the radiant coils, whose flue gases are transferred to the convection section, where energy is recovered for feed heating and steam pro-
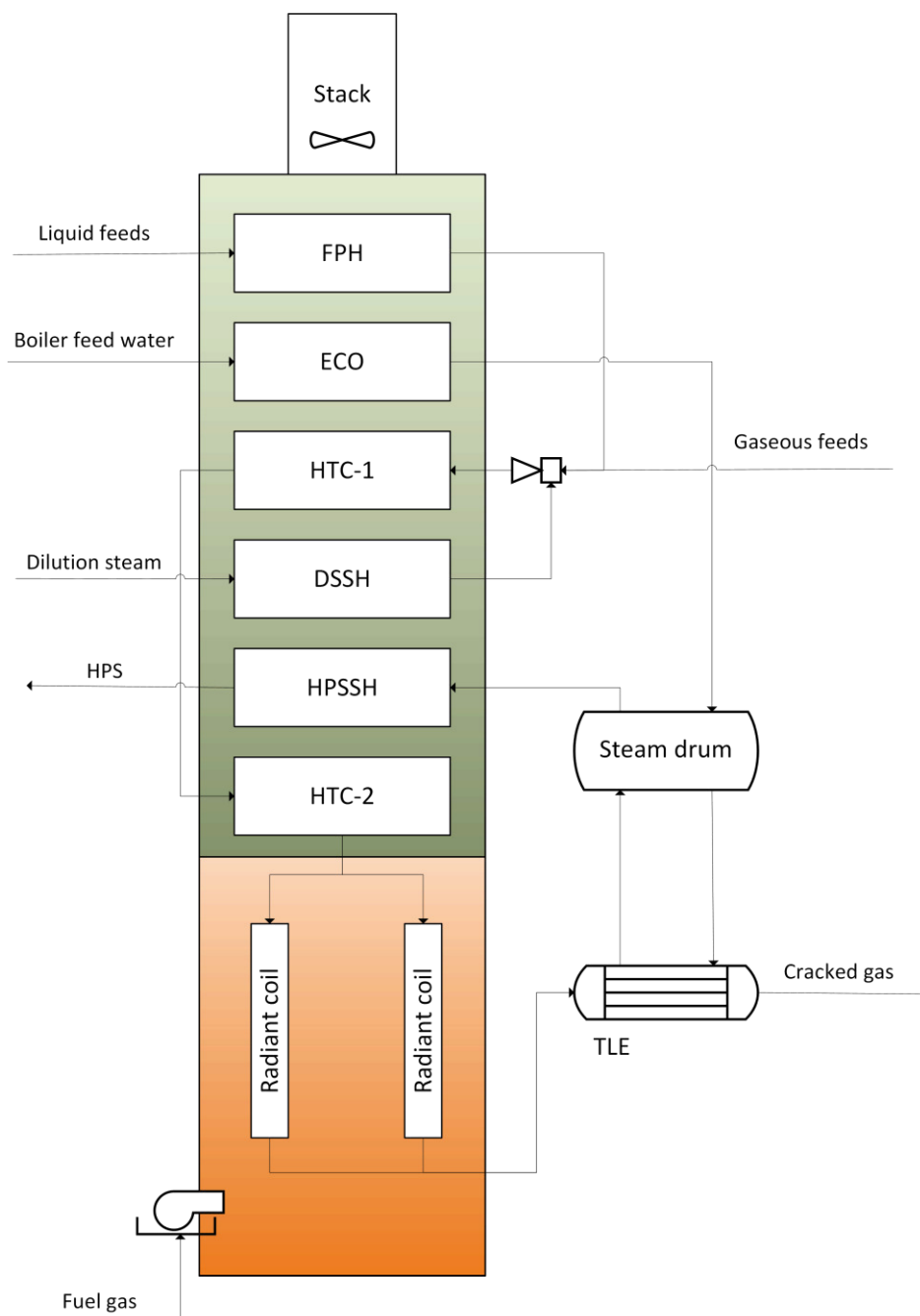

Figure 2-3: steam cracking furnace - flowchart

duction. Figure 2-3 illustrates a typical flow chart of a steam cracking furnace, indicating the convection section in green and the radiant section in orange. [2, p. 102]

The flue gas and cracking feed are processed counter-current, maximising the overall thermal efficiency of the furnace. Liquid feeds are fed at the top of the convection section to the feed preheater (FPH) where it is evaporated and superheated (typically to 150 to 300°C). Next the gaseous feed is mixed with dilution from the dilution steam preheater (DSSH, ~400°C) steam and gaseous feeds, before entering two high temperature convection sections (HTC-1 and HTC-2), where the mixture is superheated to 550° to 650°C. Finally, this mixture is fed through the cross-over to cracking coils. [2, p. 102]

Underneath the FPH the economizer (ECO) preheats the boiler feed water for high pressure steam production, before entering a steam drum. A common pressure level of HPS is 70 to 130 bar. The steam drum provides liquid for the transferline exchangers, which are operated as evaporators. The saturated steam leaving the steam drum passes a high pressure steam super heater (HPSSH), typically raising the steam temperature to 450 to 550°C. This steam is commonly used for covering the high power demand of the compression section. [2, p. 102]

The burners in the radiant box(es) are commonly operated with residue gases, typically methane with impurities like hydrogen and ethane, and an excess-air fraction of about 10%. About 40% of the burner duty is absorbed by the radiant coils, while the rest is recovered in the convection section, resulting in an overall furnace-efficiency of 90 to 95%. [2, p. 102-103]

The radiant section contains the cracking coils, acting as plug flow reactors. Typically, several coils, with varying geometries, are arranged in each firebox. Figure 2-4 shows the tube arrangement and the fields of application of available cracking coils provided by Linde. [4]
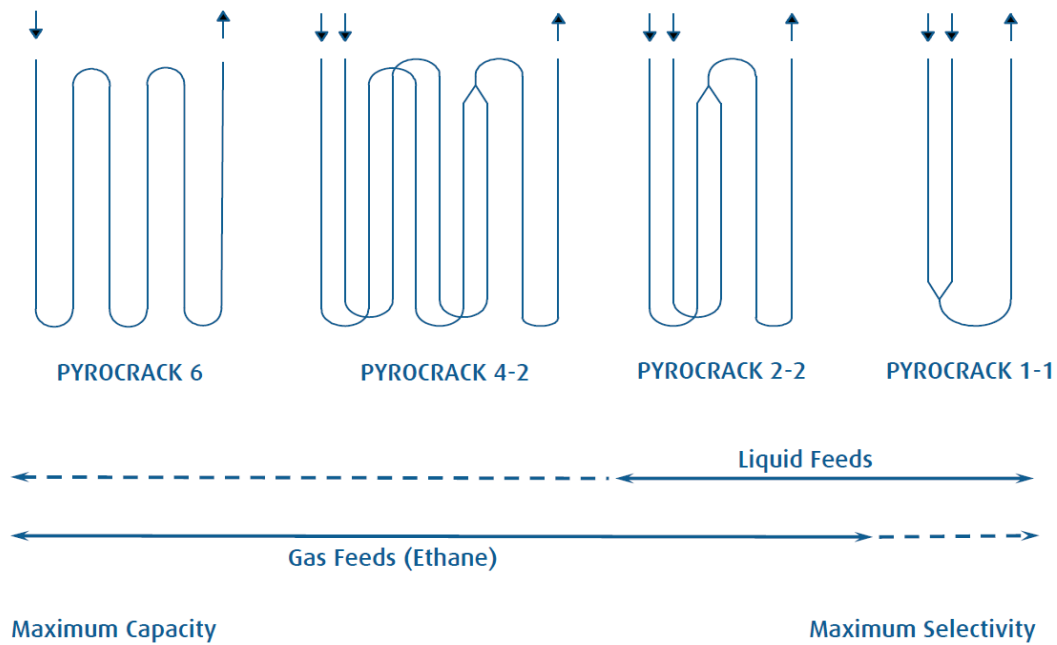

Figure 2-4: common cracking coil designs [4]

2.2   Artificial neural networks

Artificial neural networks have become widely utilized for modelling and solving many types of real-world problems in science and engineering. [5, p. 3] By now, there can be found a large variety of different types, driven by a fast development of automated data processing for big data applications like image and speak recognition. [6]

Their functional analogy to biological neural networks determines their remarkable characteristics in information processing. Their ability of learning and generalization from data provided to them, as well as featuring a high level of fault and noise toler-ance, makes them ideal for data-driven modelling. These abilities arise from the high grade of interconnection of simple neurons, which make the networks so flexible. [5, pp. 4-7]

For this work, simple multi-layer feed-forward networks are the choice for modeling the composition of steam-cracker effluents by training with simulation data.

2.2.1   The neuron

Artificial neurons (or perceptrons) are mathematically designed to act in a way like biological neurons by summing up the weighted outputs from previous neurons to use this sum as input. In nature the neuron only "fires" if the input reaches a certain level of input, this is mathematically realized by introducing a bias and feeding this biased input to an activation function. [7, pp. 10-13]

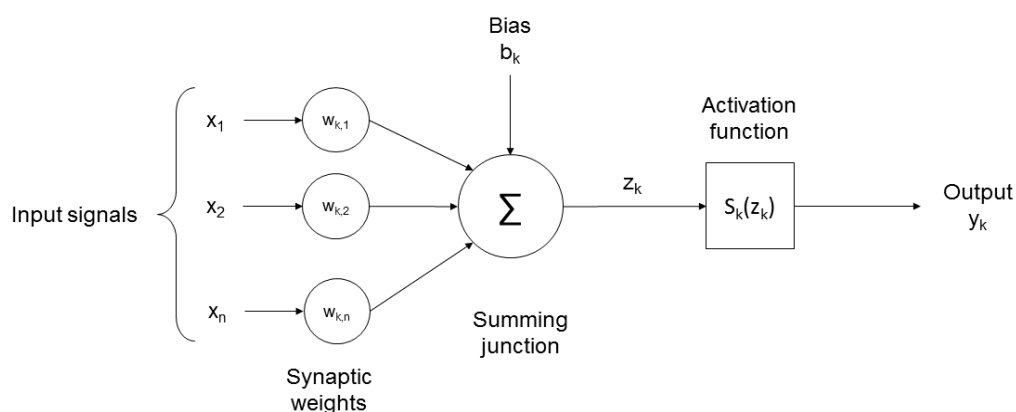Figure 2-5 shows this working principle of a neuron.

Figure 2-5: working principle of an artificial neuron

The activation function can be a step function, but in principal a logistic-sigmoid function is used, because the training algorithm needs a differentiable function. It maps a large input range to a small output of a range 0 to 1. [8, p. 403] This function is illustrated in figure 2-6.
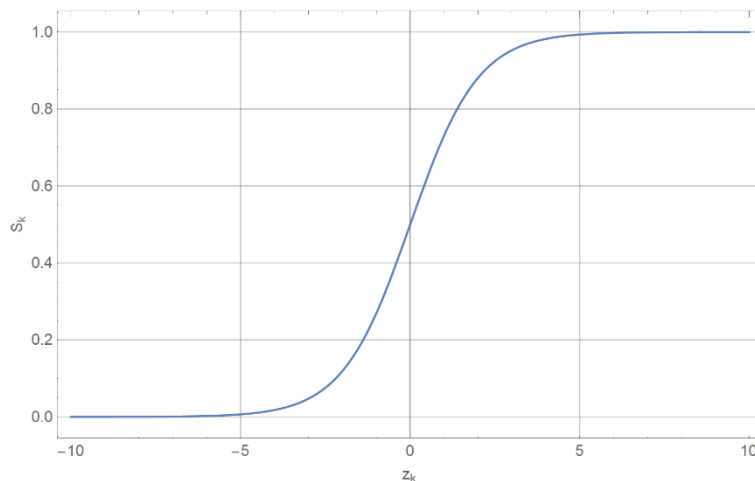
Figure 2-6: Logistic-Sigmoid Function

The summation of the weighted inputs can be written as:

$$z_k = \sum_{j=1}^{n} w_{j,k} * x_j + b_k \tag{2-1}$$

Index k denotes the neuron, fed with input variables x_j and bias b_k, resulting in the sum z_k, which is further fed to the activation function. The output of the logistic-sigmoid function then is defined as [9, p. 1543]:

$$S_k(z_k) = \frac{1}{1+\exp(-z_k)} \tag{2-2}$$

2.2.2   Feedforward networks

Feedforward networks are built up of a number of simple neurons arranged in layers, where every output of each neuron from one layer is connected to the input of each neuron of the next layer.

2.2.2.1   Single-layer feedforward networks

The simplest case of an ANN, consisting of one input and one output layer, is the so-called single-layer feedforward network, where the output layer is built up of one neuron per output in parallel. [7, p. 21] The counting of the layers starts after the input-layer, so this type counts only one layer. Such a network is illustrated in figure 2-7.
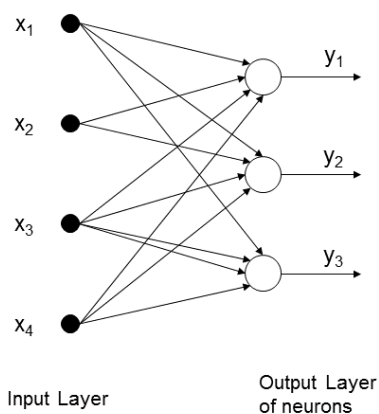

Figure 2-7: single layer feedforward network

In theory, every function can be approximated by a single-layer network, given that enough neurons are utilized. One could say, the function gets piecewise defined by the neurons, of course resulting in a poor generalization behaviour. [10, pp. 47-48]

2.2.2.2   Multi-layer feedforward networks

Multi-layer feedforward networks include hidden layers in addition to the input- and output-layer. If one hidden layer, also consisting of simple neurons in parallel, is introduced, the resulting network counts 2 layers. In figure 2-8 such a network is illustrated. By adding hidden layers, the network improves its capabilities of generalization. [9, p. 1545]
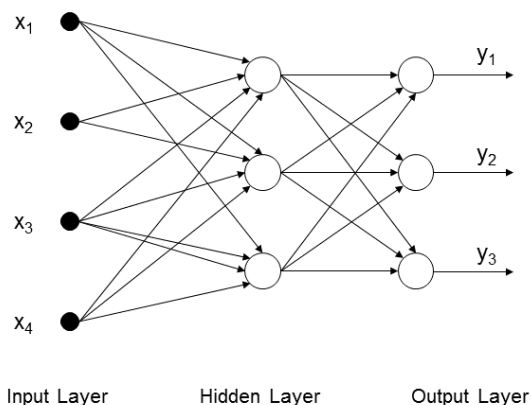
Figure 2-8: multi-layer feed-forward network

2.2.2.3   Network training

The very first step before starting to train a neural network is the initialization of its weights and biases. In most cases this is realized by setting them to small random numbers, e.g. -1 to 1 or -0.3 to 0.3. [8, p. 401]

The training of feedforward networks is done by the so called back-propagation algorithm, which has a simple workflow:

First the input tuples of the training data are fed to the network's input layer. The (initialized) network computes its output values with it, which are used to calculate the error to the output tuples of the training data. This error is propagated backward, updating weights and biases from the last to the first layer. After updating, the next iteration starts with feeding data to the network input. [8, pp. 401-407]

The used error function for each node *j* is half the sum of squared errors [7, p. 161]:

$$Err_j = \frac{1}{2} * \sum_{i=1}^{N} \left(y_{i,j} - t_{i,j} \right)^2 \tag{2-3}$$

Where $y_{i,j}$ denotes the network output and $t_{i,j}$ the targeted output data for a node j for each training tuple i of the training set N.

As convergence criteria commonly, the *SSE* - sum of squared errors [5, p. 21] or the *RMS* - rooted mean square errors [5] are utilized, defined as follows:

$$\text{SSE} = \sum_{j=1}^{N} \sum_{i=1}^{n} (y_{i,j} - t_{i,j})^2 \tag{2-4}$$

$$\text{RMS} = \sqrt{\frac{1}{N} \sum_{j=1}^{N} \sum_{i=1}^{n} (y_{i,j} - t_{i,j})^2} \tag{2-5}$$

In praxis, training is aborted after a specific training time, a specific number of training rounds or when a convergence criterion decreases to specific threshold.

2.2.2.4   Overfitting

The fact that neural networks only learn from data provided to them in training enables the possibility that they only learn to reflect the training data points, without the ability to generalize new unseen data. This phenomenon is called overfitting and correlates strongly to the chosen network topology, the bigger the network, the more susceptible it is for only learning the training data. [9, p. 1545]

To overcome this problem, it is recommended to hold back data from training and use it as a validation dataset. After each training round, the error to the training data and validation data is computed. At the beginning, the network trains well and learns to generalize, both errors will decrease, but when the network starts overfitting, the error to the validation data will start to increase, while the training error still decreases. At this point training has to be stopped, this method is called early stopping. [7, pp. 215-217]

This early stopping shall be demonstrated by training a network to reproduce the Gaussian function:

$$f(x) = e^{-x^2} \tag{2-6}$$

The training data is generated by calculating its values on the interval [-4,4] with a distance of 0.2 between the points. To imitate real measurement data, some noise, in particular normal-distributed random data with 0 mean and a variance of 0.15 is added to the smooth function. The used network is built up of one input and one output node by implication. The output layer as well as one hidden layer consist of 150 neu-

rons each. This extreme network size is chosen, to demonstrate the overfitting capabilities of neural networks.

The network is once trained for 20000 rounds only using training data, as well as once with the use of a randomly chosen 40% partition of the data as validation data. Figure 2-9 shows the resulting network behaviour, as well as the original function and the strongly scattered synthesized data for training and validation. The ANN trained without validation data learned to imitate the training data with all its noise, while the network trained with the early stopping method learned to predict a smooth curve, even though it fits not perfect the original function.
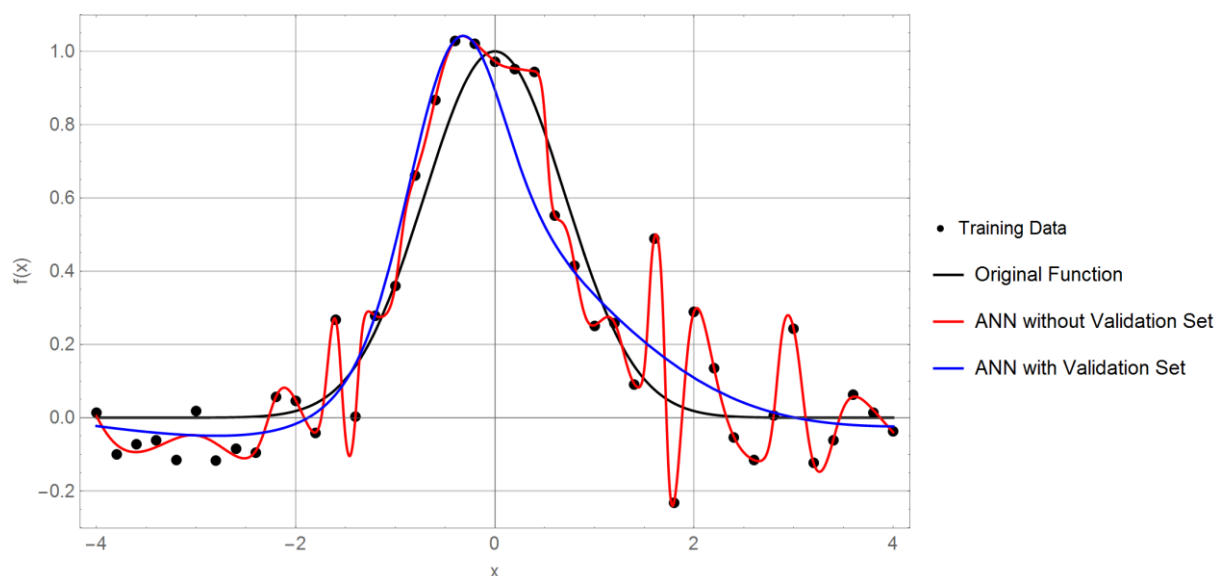

Figure 2-9: function approximation with ANN

2.3   Statistical models – linear regression

This chapter is aimed to give an overview, what kind of statistical models are commonly used to describe experimental data and how linear regression works. Detailed information about statistical preconditions and mathematical derivations of linear regression and statistical modelling can be found in [11].

2.3.1   Regression models

In general, linear regression models can be classified how the predictor variables (X_i) influence the response variables (Y) leading to the following model types [12].

2.3.1.1   Simple linear regression model

The most common model used for regression issues is the formula of a straight line, describing the data with one predictor variable. Its variables are the slope and the intercept.

$$Y = b_0 + b_1 * X \tag{2-7}$$

2.3.1.2   Multiple linear regression model

In case there exist more than one predictor variable (X_1, X_2 … X_n), the model can be extended to the following form:

$$Y = b_0 + b_1 * X_1 + b_2 * X_2 \cdots b_n * X_n \tag{2-8}$$

Such a model does not account for interaction between predictor variables itself.

2.3.1.3   General linear regression - polynomial regression

For both previous model types, the linear form of the response variable can be extended to a polynomial form (here the case of one predictor variable is presented) [12]:

$$Y = b_0 + b_1 * X_1 + b_2 * X_1^2 \tag{2-9}$$

This is mathematically done by substitution:

$$Z_1 = X_1 \ and \ Z_2 = X_1^2 \tag{2-10}$$

Resulting in a pure linear function:

$$Y = b_0 + b_1 * Z_1 + b_2 * Z_2 \tag{2-11}$$

This type with several predictor variables will later be used for the regression of the simulation data. In the case of 3 predictor variables and the use of quadratic polynomials, the model looks like:

$$Y = b_0 + b_1 * X_1 + b_2 * X_1^2 + b_3 * X_2 + b_3 * X_2^2 + b_4 * X_3 + b_5 * X_3^2 \qquad (2\text{-}12)$$

2.3.1.4   General linear regression - interaction coefficients

All previous regression models offer only consideration of independent predictors. By introducing interaction parameters between the predictor variables, this problem can be overcome. Such a model of 2 predictor variables with quadratic polynomials and one interaction parameter has the following form:

$$Y = b_0 + b_1 * X_1 + b_2 * X_1^2 + b_3 * X_2 + b_3 * X_3^2 + b_5 * X_1 * X_2 \qquad (2\text{-}13)$$

2.3.2   Least squares method

The least squares method minimizes the quadratic error between the data and regression model by adjusting the parameters of the model. In the following Y_i denotes the Y from data and $\hat{Y}$ the model response. [12]

$$\sum_{i=1}^{n}\left(Y_i - \hat{Y}\right)^2 \rightarrow min \qquad (2\text{-}14)$$

In case of linear regression, a closed form for this minimisation exists, resulting in a straight-forward and fast calculation. By writing the model in matrix form (see. 2-15 and 2-16), a general formula for this method can be provided (2-17).

Arranging the data in matrix form has to be done in this way, n denotes the number of data points and $p\text{-}1$ is the number of model parameters:

$$\mathbf{X}_{n \times p} = \begin{bmatrix} 1 & X_{11} & X_{12} & \ldots & X_{1,p-1} \\ 1 & X_{21} & X_{22} & \ldots & X_{2,p-1} \\ \vdots & \vdots & \vdots & \ldots & \vdots \\ 1 & X_{n1} & X_{n2} & \ldots & X_{n,p-1} \end{bmatrix} \qquad (2\text{-}15)$$

$$\mathbf{Y}_{n \times 1} = \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{bmatrix} \qquad (2\text{-}16)$$

The model parameters are calculated with:

$$\mathbf{b}_{p\times 1} = \begin{bmatrix} b_0 \\ b_1 \\ \vdots \\ b_{p-1} \end{bmatrix} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}$$

(2-17)

3 Model development

The target of this work is the development of fast-computing black-box models, which can predict the cracked gas composition at the coil outlet of every single steam cracking furnace of the considered ethylene plant. This chapter describes the workflow of data generation, data handling and data pre-processing to reactor model development. As resulting reactor models, neural networks and classical polynomials are trained, respectively fitted.

3.1 Design of experiment

As already described in 2.1.3, the cracked gas composition of a steam cracker depends on the feed mass flow as well as its composition, the dilution steam ratio and the temperature at the coil outlet. This knowledge makes a more or less complicated predictor analysis dispensable. Additionally, several furnaces show the same feed selection and coil geometry, so some models can be used for more than one furnace.

The data basis for the models is generated by radical kinetic simulation of the radiant section of the cracking furnaces, which makes a design of experiment indispensable. First, the boundaries for each predictor variable are set and then discrete equidistant values on this interval are chosen. With this set of ranges, a set of all combinatorically possible cases is calculated.

Handling the mass flow rate and its composition is realized as simply using the mass flow rate of each discrete feed type as a predictor variable. This step would let the number of possible cases explode, if the total sum of feed mass flows is not limited. By analysing the compositions of the possible feed streams of the plant, the following possible mass flow rates can be introduced as predictor variables of the particular cracking furnaces:

Ethane, Propane, n-Butan, iso-Butan, C4-Mix
Naphta 1, Naphta 2, Naphta 3, Naphta 4

Of course, not all of them can be processed by a single furnace, so each model has less than the sum of these feed predictors. In addition to the feed mass flows, the values of the COT as well as the steam dilution ratio are introduced as predictor vari-

ables. To determine to necessary ranges for the predictor variables, historical opera-
tion data of the feed management system and the cracking furnaces of the last 1.75
years is analysed.

Considering the operating ranges and different coil geometries, a resulting set of 6
different reactor models can be determined. The number of different values in each
dimension (in each predictor) is set in a way, that it is high enough to provide enough
data for generalization on one hand and, on the other hand, to keep the simulation
time of the total number of cases as low as possible. An overview of the resulting
case-set for each reactor model simulation is shown in table 3-1 and table 3-2.

Table 3-1: design of experiment – 1/2

reactor model	1	2	3
furnace	1	2,3,5,6	4
naphta 1 [t/h]			
naphta 2 [t/h]	0, 3, 6, 9, 12, 15, 18, 21, 24	0, 6, 12, 18, 24	0, 5, 10, 15, 20, 25
naphta 3 [t/h]	0, 3, 6, 9, 12, 15, 18, 21, 24, 27	0, 6, 12, 18, 24	0, 5, 10, 15, 20, 25
naphta 4 [t/h]	0, 3, 6, 9, 12, 15, 18, 21, 24, 27, 30		
C4-mix [t/h]		0, 3, 6, 9, 12	0, 3, 6, 9, 12, 15
Ethane [t/h]		0, 3, 6, 9	
Propane [t/h]		0, 3, 6, 9	0, 3, 6, 9
n-Butane [t/h]		0, 3, 6, 9	0, 3, 6, 9
iso-Butane [t/h]		0, 3, 6, 9	0, 3, 6, 9
COT [°C]	760, 780, 800, 820, 840, 860	800, 820, 840, 860	780, 800, 820, 840, 860
steam diltion ratio [t/t]	0.35, 0.45, 0.55, 0.65	0.4, 0.5, 0.6	0.4, 0.5, 0.6
feed constraint [t/h]	12 < sum <= 30	15 <= sum <= 26	16 <= sum <= 25
number of cases	5.904	21.180	14.295

Table 3-2: design of experiment - 2/2

reactor model	4	5	6
furnace	7	8	9,10
naphta 1 [t/h]			20, 22, 24, 26, 28, 30, 32, 34
naphta 2 [t/h]			
naphta 3 [t/h]			
naphta 4 [t/h]			
C4-mix [t/h]	0, 3, 6, 9, 12, 15		
Ethane [t/h]	0, 3, 6, 9, 12	3, 4, 5, 6, 7, 8, 9, 10, 11, 12	
Propane [t/h]	0, 3, 6, 9		
n-Butane [t/h]	0, 3, 6, 9		
iso-Butane [t/h]	0, 3, 6, 9		
COT [°C]	820, 840, 860	760, 780, 800, 820, 840, 860	760, 780, 800, 820, 840, 860
steam diltion ratio [t/t]	0.35, 0.45, 0.55, 0.65	0.3, 0.4, 0.5, 0.6	0.35, 0.4, 0.45, 0.5, 0.55
feed constraint [t/h]	12 < sum <= 22		
number of cases	5.688	240	240

3.2   Data handling and simulation

For each reactor model design of experiments and with this, possible case tuples are calculated with Wolfram Mathematica. Also, the manipulation of the XML-files, as input files for the kinetic simulation, as well as the extraction of the results are realized with Mathematica. For each case a XML file is generated, which results in several thousand simulation files. An automated case simulation handler is programmed as an EXCEL file, which looks up the current directory for all XML files and runs them one by one. Additionally, it generates so-called hot-start-files, which include start values for 1D-simulation, minimizing the simulation time drastically from 30 to 60 seconds to 3 to 20 seconds per simulation. For that, one hot start file is generated manually by running a simulation of any case of the particular reactor model. Another feature of the EXCEL-XML-handler is its XML-parser, which opens each file after its simulation and checks the convergence status. The reason for that is, some cases (about 15 out of 10.000) do not converge due to bad start values from the hot-start-files. Those hot-start-files can be deleted and the cases re-run also automatically, resulting in a completely converged set of simulation files.

A Mathematica Script then reads out the whole folder of converged XML cases and writes the resulting reactor effluent (mass fractions on wet basis) compositions to a dataset, which is processed in the further steps.

Wet basis means, that the effluent composition includes the dilution steam, therefore these compositions are not very meaningful. Calculating the composition on dry basis makes the result more comparable. This is simply done for each simulation case by use of formula 3-1, where i denotes the component and j the case.

$$x_{i,j_{dry}} = \frac{x_{i,j_{wet}}}{1-x_{H2O,j_{wet}}} \tag{3-1}$$

This is the very first step of data pre-processing for both model types, so the following compositions are always on dry basis.

3.3   Component filter

The component list used by the simulation program includes more than 120 components, by calculating the dry basis already one gets eliminated. These components include a few gases and mainly hydrocarbons, ranging from methane to a C40-hydrocarbons. A rule of thumb says, that steam cracking of light hydrocarbons and naphtas will not produce that heavy hydrocarbons, so the component list can be filtered to reduce the final model size.

Therefore, the whole dataset of dry reactor effluents (of a specific reactor model) is looked up for the maximum occurring value of each component. By comparing these values with a specific threshold, the component list can be reduced to components, whose values never fall below the threshold.

For each reactor model the threshold is varied in a range from 10^{-1} to 10^{-10}. Figure 3-1 shows a bar chart illustrating the number of remaining components after filtering with this threshold range. To a threshold of 10^{-4} the increase number of components is quite steep.

This is done for all reactor types and a threshold of 10^{-3} for the reduction of the component list is selected. This value of 0.1% is considered to be sufficiently accurate for the application of these reactor models.
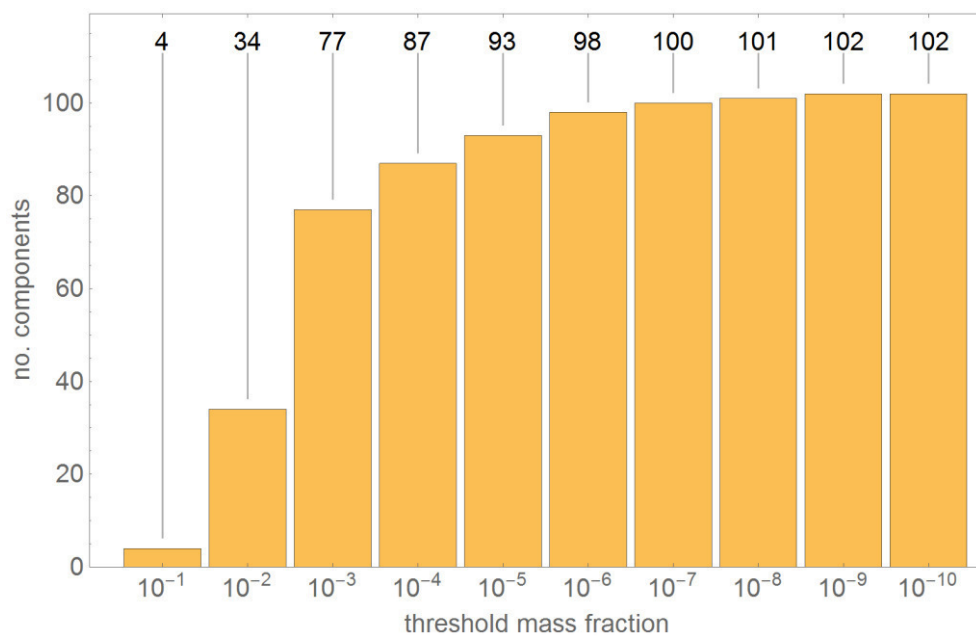

Figure 3-1: number of remaining components after filtering
(reactor model 1)

3.4   Neural network models

Wolfram Mathematica comes with a very powerful neural network package, offering a large toolbox for applications ranging from simple classification and feed forward networks to image classification and speech recognition. Thus, this toolbox is utilized for development and training neural networks for modelling the reactor effluent composition.

Developing a neural network for a particular reactor is done by the following workflow:

1. Import of dry reactor effluent compositions (as model outputs) and design of experiment data (as model inputs)

2. Filter reactor effluent components

3. Generate training data: Transform input and output data

4. Select a network topology (begin with small networks)

5. Randomize training data

6. Train network with cross-validation

7. Check prediction performance

    a) If too low → go to 4 and select an larger topology

8. Create package with ANN and transformation functions for inputs and outputs

3.4.1   Data transformation

An important precondition for training neural networks is, that all input and output values are of a similar dimension, which is not fulfilled by the training data. The input datas' dimension (mass flows, COT, steam dilution ratio) ranges 10^{-1} to 10^{3}, as well as the output datas' dimension ranges from 10^{-3} to 10^{-1}.

Transforming the input as well as the output data influences the training speed as well as the resulting ANN dramatically. Several possibilities for transformation, depending on the particular distribution, are suggested by [9] and [5]. For this work, a simple linear transformation turned out to be sufficient. Intuitively, the boundaries for the interval would be chosen like 0 to 1, but it is said to get better results by scaling the data to a slightly offset interval, like 0.1 to 0.9. [9, p. 1547]

The linear transformation is carried out for each value i to the interval $[b_1, b_2]$ of every input and output parameter j, using function 3-2:

$$t_{j,i} = b_1 + (b_2 - b_1) * \frac{x_{j,i} - x_j^{min}}{x_j^{max} - x_j^{min}} \tag{3-2}$$

Where t_{ji} denotes the resulting transformed value.

For later back-transforming of ANN results, it is necessary to store the values of $x_{j,min}$ and $x_{j,max}$. The formula for this, 3-3, can be analogously derived:

$$x_{j,i} = x_j^{min} + \left(x_j^{max} - x_j^{min}\right) * \frac{t_{j,i} - b_1}{b_2 - b_1} \tag{3-3}$$

To investigate the effect of different scaling strategies to the training result, a training of the ANN model of reactor 1 is carried out with the normal training parameters for 5000 rounds, but varying the scaling ranges. The chosen data transformations are a scaling to the intervals [0,1] and [0.1, 0.9] as well as only transforming the input data to the unit interval [0,1]. The result in form of a plot of the RMS error over the training rounds is shown in figure 3-2.

While the training progresses of datasets scaled to [0, 1] and [0.1, 0.9] are obviously not differing, it seems that the dataset with the unscaled output data trains much faster. The reason for that can be found in the way that the RMS error is calculated. The training algorithm only "sees" the data provided to it, therefore the error is also

scaled. By back-transforming the network results, an unscaled RMS error can be calculated. This is done for the resulting networks without recording the training progress, shown in figure 3-3.

Figure 3-2: effect of data scaling on network training
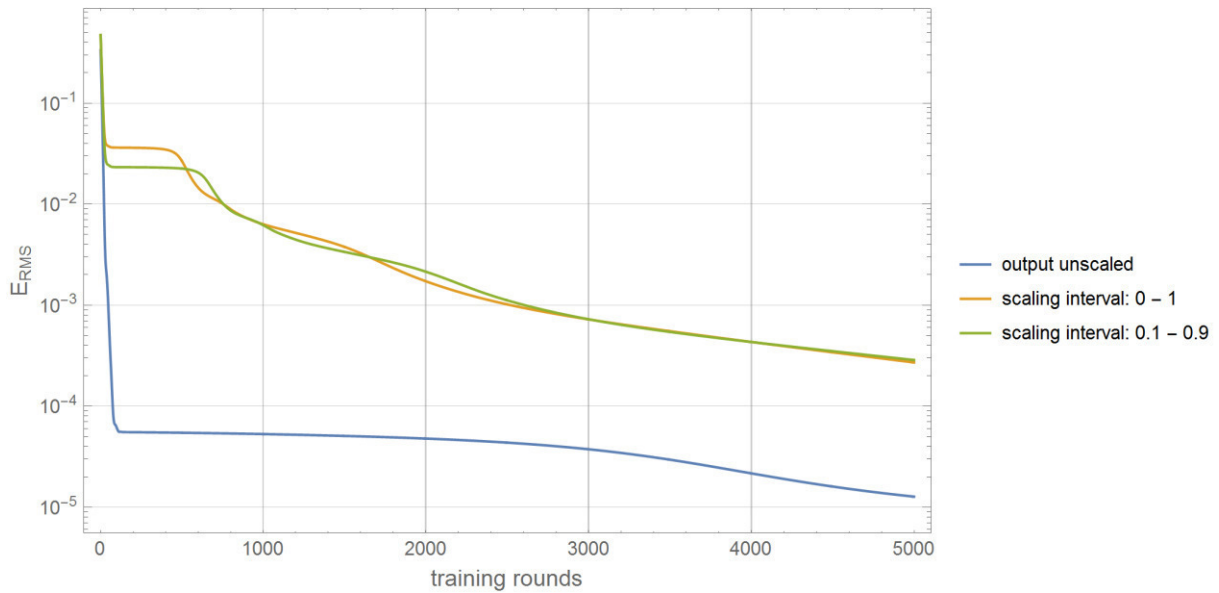
The results show, that the training with unscaled output data shows a poor performance, while both other training methods perform nearly identically. Due to the recommendation in literature and this investigation, further network training is carried out with a dataset scaling to the interval [0.1, 0.9].

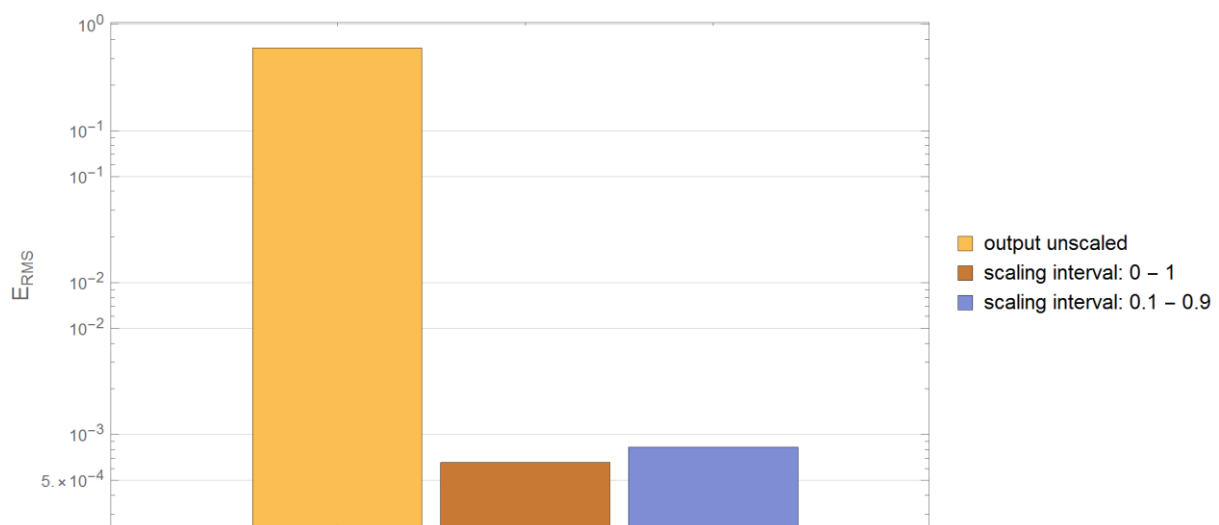

Figure 3-3: unscaled RMS error for different data scaling methods

3.4.2   Network design and training

The topology of the neural networks has to be chosen before it can be initialised and trained with data. The number of input-ports and the number of neurons in the output layer is defined by the number of input and output-variables of the resulting model, therefore only the size and number of the hidden layers can be varied.

There is no "right" way respectively no standard procedure to determine the number of hidden layers as well as the number of hidden neurons. In [5, pp. 22-23] several formulas for estimation of the number of hidden neurons are summarized. Two of them (see 3-4 and 3-5) can be applied for the reactor models in this work. N_{HN} denotes the number of hidden neuron, N_{TRN} the number of training patterns, in particular the number of different simulation cases for the model, N_{IN} and N_{OUT} the number of Input and output ports of the network.

$$N_{HN} = \frac{N_{TRN}}{5*(N_{In}+N_{Out})} \tag{3-4}$$

$$N_{HN} = \sqrt{N_{In} * N_{Out}} \tag{3-5}$$

These formulas give a first estimation of the required number of hidden neurons, the final sizing is a very empirical process and is done by trial and error by increasing the number of hidden neurons until the RMS error of the training is considered small enough.

As already stated in 2.2.2.2, the generalization performance of an ANN increases with the number of hidden layers. For this reason, the optimal number of hidden layers is found to be generally 3 for the particular problem. A further increase of this number did not lead to a better performance of the neural models, except reactor model 2, which involves highest number of predictor variables and showed a better performance with 4 hidden layers. In table 3-3 the resulting topology of the reactor models can be found.

Table 3-3: network topology of developed reactor models

Reactor model	Input-ports	Hidden layer 1	Hidden layer 2	Hidden layer 3	Hidden layer 4	Output layer
1	5	35	60	77	-	77
2	9	35	40	53	53	53
3	8	45	60	60	-	60
4	7	37	74	74	-	37
5	3	15	24	24	-	24
6	3	25	55	73	-	73

3.4.2.1   Training and algorithms

Network training with the back-propagation algorithm is realized in Mathematica with the *NetTrain*-Function. It is responsible for training as well as cross-validation and is able to run the training on several CPU-cores or GPUs in parallel.

There are three different optimizing algorithms (used for back-propagation) available when calling the NetTrain-Function, namely the SGD, RMSProp and ADAM algorithms. The last is approved to be the most suitable by [6].
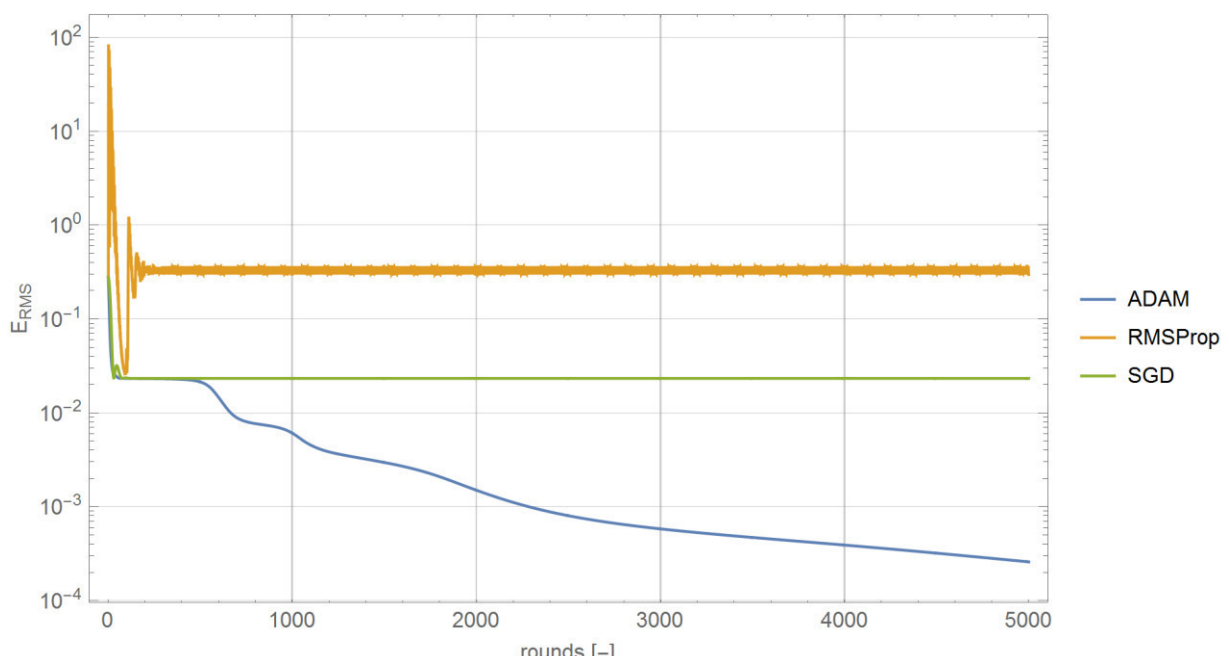

Figure 3-4: comparison of training algorithms

For selecting the most suitable for the particular applications, these three algorithms are compared by training the ANN model for reactor 1 with them. In figure 3-4 the resulting training progress is plotted over the training rounds. It is obvious that the ADAM algorithm performs best, while the SGD algorithm apparently gets stuck in a local optimum and the RMSProp algorithm is oscillating at a high RMS error level. Therefore, the ADAM algorithm is chosen for further network training.

3.4.2.2   Batch-size

Network training can be done by presenting the training tuples to the network one by one or in batch-mode, which influences how often the network weights are updated. Batch mode is more likely to get trapped in a local optimum, so reducing the batch size to 1 can improve the training result. [9, p. 1549]

Hence one training round consists of processing the training data set one time, the time consumed for one training round decreases with increasing batch size. But, this does not implicate that a large batch size results in a faster training speed. Literature states, that training with "mini-batches" results in the highest training speed. [6]

To determine the optimal batch size, the batch size for training of the ANN model of reactor 1 is varied from 1 to the size of the whole training set (5904), and each training is run for exactly 60 seconds. The resulting training progress is plotted in figure 3-5, thus it appears that a batch size of 10 to 100 lets the algorithm perform best.
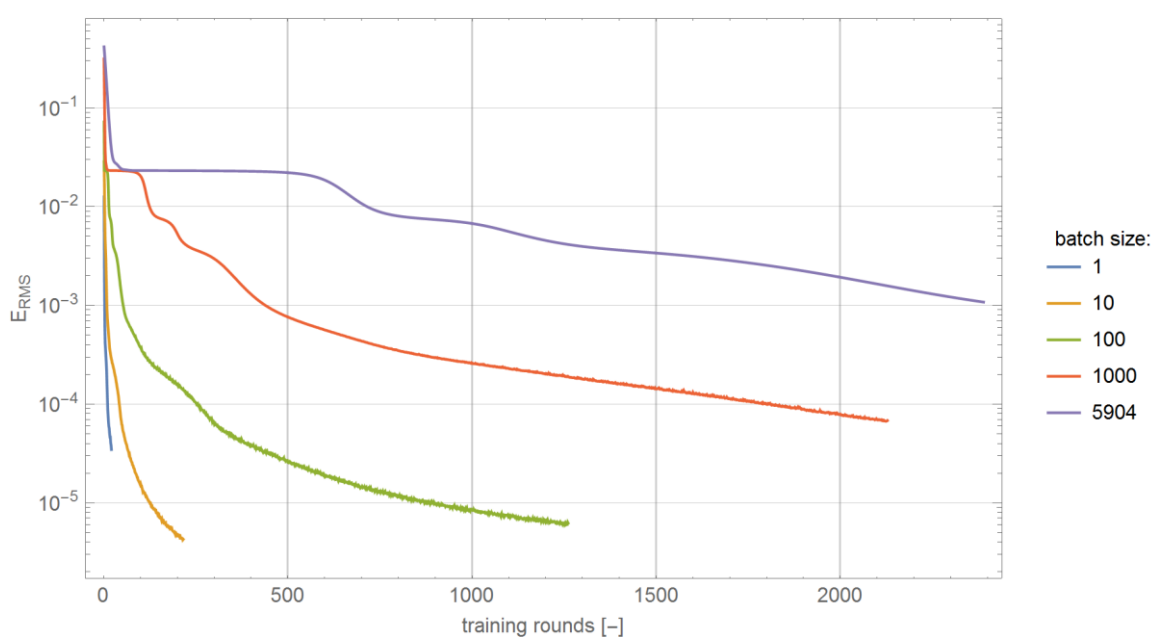
Figure 3-5: RMS error evolution for 1 minute training with different batch sizes

3.4.2.3   Cross validation

To avoid overfitting, a partition of 33,33% of the generated data by simulation is se-lected for validation, thus a large part of data for training would get lost. To overcome this problem, a so-called k-fold cross-validation is performed, in particular this results in a 3-fold cross-validation. Thereby, the dataset is divided into k partitions and net-work training is performed with the validation-dataset k and the remaining partitions are used for as training datasets. By repeating this procedure several (n) times, all partitions get used as validation datasets n/k times. Figure 3-6 illustrates this method.
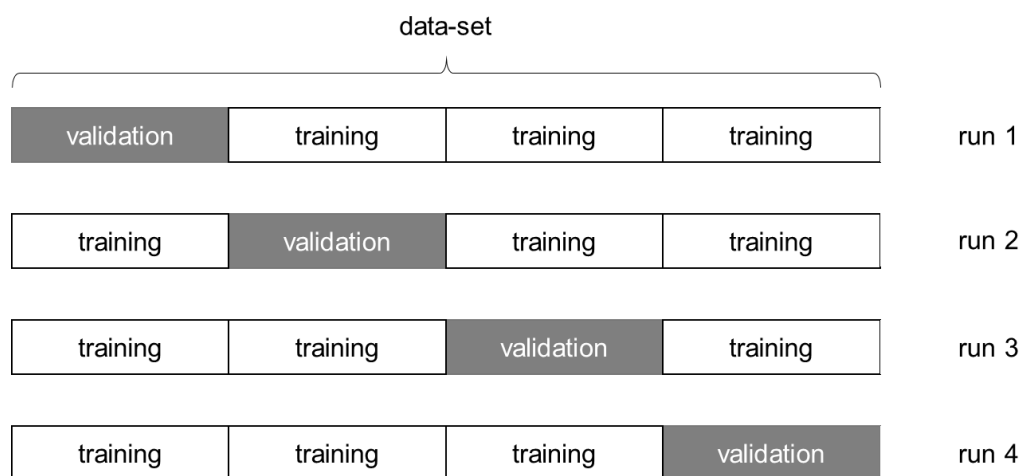
Figure 3-6: cross validation

Practically, every 10^4 to $3*10^4$ training rounds the validation set is changed to the next one, while the total sum of training rounds is in the range of $6*10^4$ to $2.1*10^5$, thereby this procedure is repeated several times.

3.4.2.4   Training progress and convergence criterion

The training is stopped after reaching a RMS error of about 10^{-6}, which is often found to be the lower limit when training for very long time. Figure 3-7 shows the asymptotic training trend as well as the course of the error to the training data.
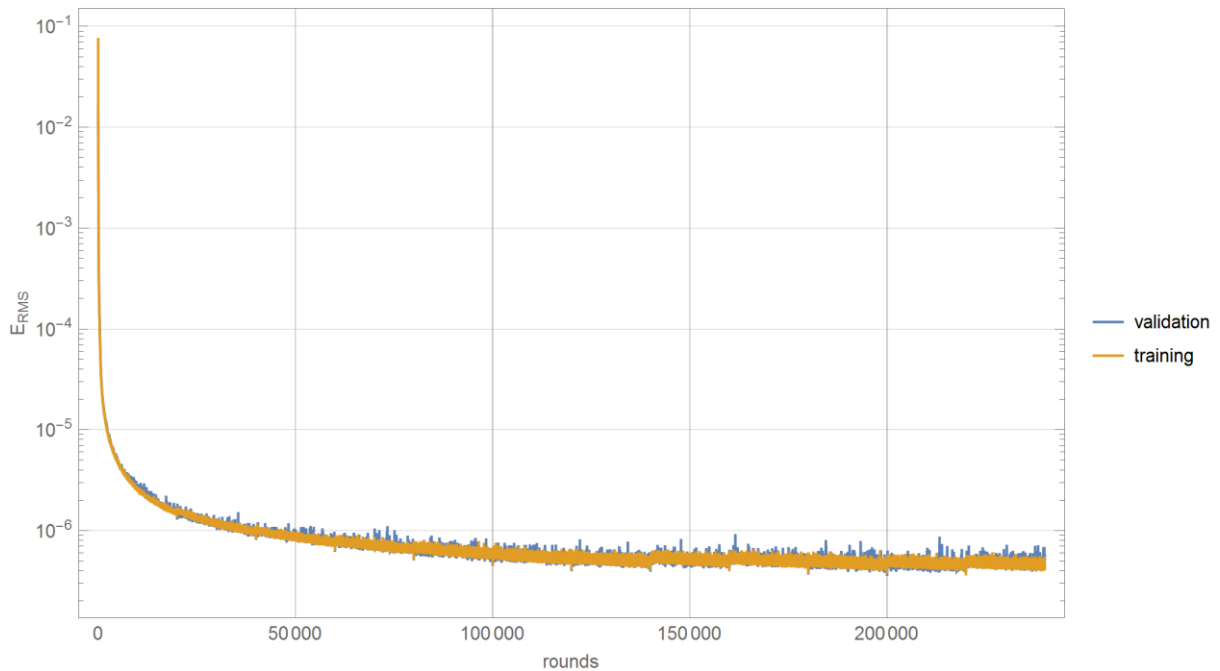
Figure 3-7: training progress of reactor model 3

Due to the noise-free and smooth training data provided to the network, the network is not tending to over-fit.

3.5 Function fitting

As a different modelling approach, sets of classical polynomials are fitted with the same datasets as already used for the neural network models. The model boundaries are completely the same as those of the ANN reactor models, so the models can be exchanged easily in further calculations. Such a reactor model is built up of a set of functions, each function describing the dry mass fraction of one component. All input parameters are selected as predictor variables of the function, these are the feed mass flows, COT and steam dilution ratio. This approach is carried out with quadratic and cubic polynomials, whose functions are exemplarily shown in (3-6) and (3-7) for a reactor with two feed mass flows.

$$Y_{i,quadratic} = C_1 + C_2 * MF_1 + C_3 * MF_1^2 + C_4 * MF_2 + C_5 * MF_2^2 + C_6 * COT +$$
$$C_7 * COT^2 + C_8 * STR + C_9 * STR^2 \tag{3-6}$$

$$Y_{i,cubic} = C_1 + C_2 * MF_1 + C_3 * MF_1^2 + C_4 * MF_1^3 + C_5 * MF_2 + C_6 * MF_2^2 + C_7 *$$
$$MF_2^3 + C_8 * COT + C_9 * COT^2 + C_{10} * COT^3 + C_{11} * STR + C_{12} * STR^2 + C_{13} * STR^3 \tag{3-7}$$

Y_i denotes the dry mass fraction of component i, the predictors MF, COT and STR are the values of the feed mass flows, coil outlet temperature and steam dilution ratio, while the constants C are adjusted by the least-square-method.

The fitting of polynomial functions is performed by the *LinearModelFit*-Function in Mathematica, running the least-square-method described in 2.3.2. For every reactor model the fitting is performed for each of its previously filtered components one by one. This results in large sets of functions and their coefficients, which are hard to handle manually. Tables with the fitted coefficients for all reactor models and their functions can be found in 6.1.

4 Validation and comparison to measurements

The developed reactor models must be validated to check their prediction abilities and precision. Therefore, three historical plant production cases are selected in a way, that the reactor parameters are as different as possible. To get reference values for comparison, the reactor effluent compositions of these three scenarios are calculated by kinetic simulation. Additionally, data from on-line measurements of the ethylene plant is used for comparison with the black box models and the kinetic simulations. These on-line measurements include mass fractions of the key components of each furnace's cracked gas composition.

The historical production data of the feed management system and those for all steam cracking furnaces are exported from the process control system of the plant. With these data, kinetic simulation data and input data for the black box models are obtained. Table 4-1 to table 4-3 summarize the process data for each of the three reference scenarios.

Table 4-1: process data - case 1

furnace	1	2	3	4	5	6	7	8	9	10
reactor model	1	2	2	3	2	2	4	5	6	6
naphta 1 [t/h]									27,95	28,10
naphta 2 [t/h]	0									
naphta 3 [t/h]	0	7,01	6,32	15,50	13,52	15,29				
naphta 4 [t/h]	0									
C4-mix [t/h]		1,84	2,00	4,22	6,27	5,38	0			
Ethane [t/h]		2,17	2,71		0,00	0,00	0	9,01		
Propane [t/h]		4,13	5,09	0,35	0,51	0,44	0			
n-Butane [t/h]		5,43	5,26	1,51	2,25	1,93	0			
iso-Butane [t/h]		2,65	2,63	0,41	0,61	0,52	0			
COT [°C]		855,2	855,1	845,3	835,2	850,2		850,1	855,2	855,3
steam dilution ratio [t/t]	0	0,49	0,45	0,54	0,43	0,44	0	0,357	0,40	0,40

Table 4-2: process data - case 2

furnace	1	2	3	4	5	6	7	8	9	10
reactor model	1	2	2	3	2	2	4	5	6	6
naphta 1 [t/h]									28,38	28,64
naphta 2 [t/h]	0									
naphta 3 [t/h]	0	7,87	6,59	13,01	8,65	11,04				
naphta 4 [t/h]	0									
C4-mix [t/h]		0,00	0,00	6,83	9,24	10,16	0			
Ethane [t/h]		1,26	1,58		0,00	0,00	0	9,00		
Propane [t/h]		5,58	6,88	0,29	0,39	0,43	0			
n-Butane [t/h]		5,22	4,85	1,05	1,41	1,56	0			
iso-Butane [t/h]		2,81	2,76	0,33	0,45	0,50	0			
COT [°C]		850,0	855,0	849,6	835,9	848,4		850,1	854,9	855,2
steam dilution ratio [t/t]	0	0,45	0,46	0,45	0,53	0,41	0	0,36	0,40	0,40

Table 4-3: process data - case 3

furnace	1	2	3	4	5	6	7	8	9	10
reactor model	1	2	2	3	2	2	4	5	6	6
naphta 1 [t/h]									27,91	28,30
naphta 2 [t/h]	0									
naphta 3 [t/h]	19,71	0	10,57	13,01	14,04	13,61				
naphta 4 [t/h]										
C4-mix [t/h]		0	1,68	7,00	6,81	6,62	2,66			
Ethane [t/h]		0	1,75		0,00	0,00	8,03	9,00		
Propane [t/h]		0	2,72	0,46	0,44	0,43	4,07			
n-Butane [t/h]		0	4,47	2,00	1,94	1,89	1,58			
iso-Butane [t/h]		0	2,13	0,54	0,53	0,51	0,91			
COT [°C]	840,0		855,0	845,0	835,0	850,0	840,1	850,1	855,3	854,8
steam dilution ratio [t/t]	0,58	0,00	0,45	0,46	0,42	0,45	0,42	0,36	0,41	0,41

4.1   Degree of polynomials

The reactor models based on polynomials utilize quadratic and cubic approaches for regression. The cubic polynomials offer one parameter per predictor more than the quadratic ones, so these should result in a better fit performance. Instead of looking at R^2-values, which only give information, how well the function fits the training data, the two approaches are directly compared to unseen data from the three validation cases.
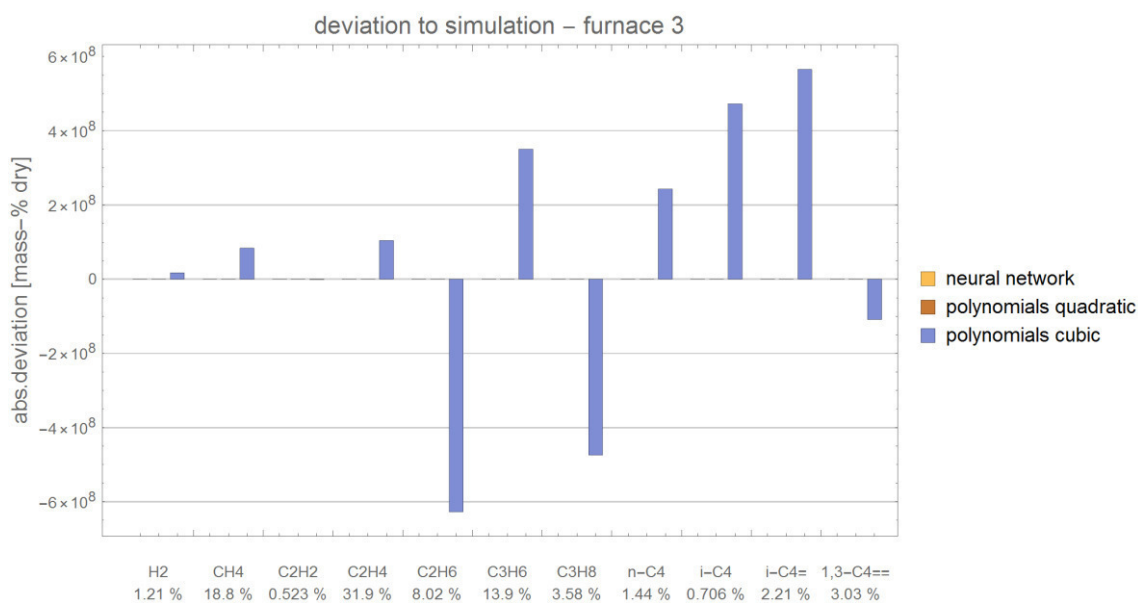

Figure 4-1: abs. deviation to simulation of polynomials - furnace 3 (case 1)

As can be seen in figure 4-1, the cubic polynomials show an extremely high deviation to the simulation data, while they perform the same as the quadratic ones in figure 4-2. The reason for that is the different number of predictor variables. A high number of predictor variables leads to an even higher number of fitted constants, giving the functions the possibility for overfitting and results in bad generalization capabilities. Thus, the cubic polynomials show no overfitting for furnace 9, where the number of predictor variables is low with three, whereas the deviation for furnace 3 is extremely high, due to high number of predictor variables (9).

Another finding is, that the cubic fit never performs better on the test scenarios than the quadratic ones, leading to the decision of dropping the cubic approach.
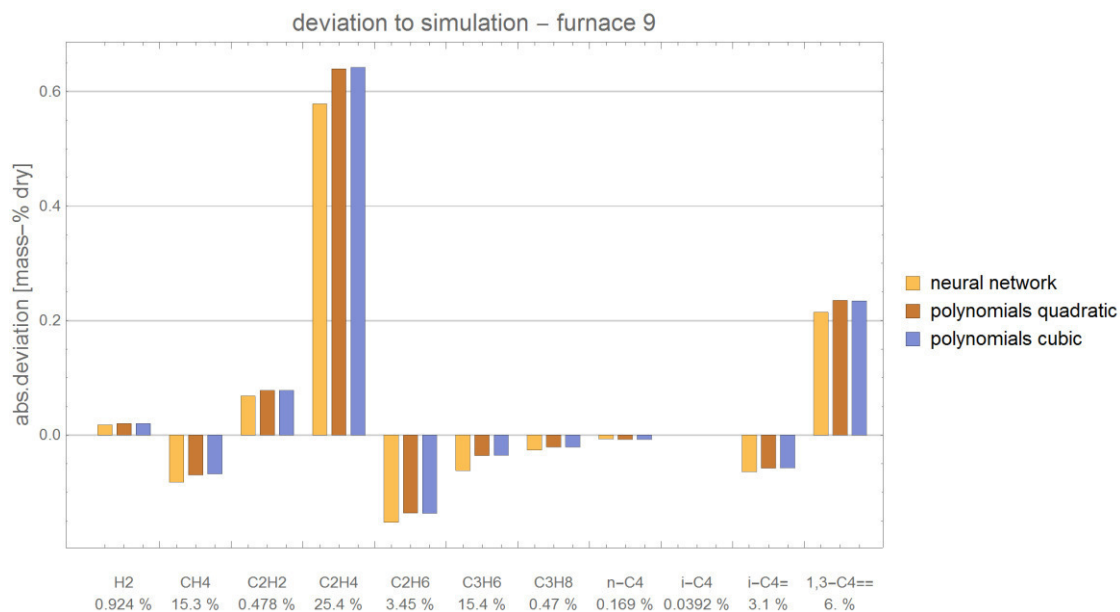
Figure 4-2: abs. deviation to simulation of polynomial - furnace 9 (case 1)

4.2   Model deviations to simulation

4.2.1   Reactor models

In this chapter the performance of both modeling approaches for each reactor, neural network models and the quadratic polynomial models, are evaluated by comparing the mass fractions of the models with those from the simulations of the validation cases. As comparison basis absolute deviations of the dry mass fraction are chosen, because the compared key components are ranging from nearly zero to about 50%, resulting in low relative deviations for the important components ethylene and propylene, whereas the relative deviations for components occurring in traces, like n-butane, would explode. This comparison is done for all furnaces and all reference cases, for each furnace an example is listed here. Due to the lack of large differences in the results between the three validation cases, the remaining comparisons are listed in 6.2. The numbers below the component names denote the simulated values of these components.

4.2.1.1   Reactor model 1

These reactor models calculate the cracking of three naphtas, without co-cracking of light gases. Figure 4-3 shows the deviations of the neural network model and the polynomial model, both performing well. The neural network's maximum deviation is 0.25%, while the polynomial fit is much higher at a level of 0.65%, which is outstanding for this simple fit method applied to such a complex problem.
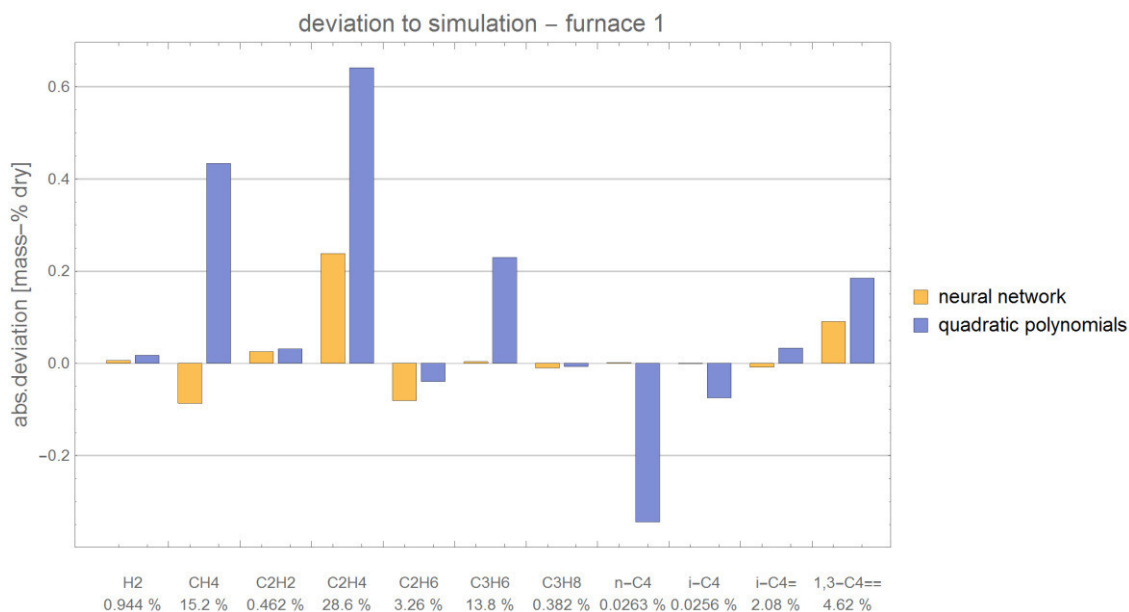
Figure 4-3: abs. deviation to simulation - furnace 1 (case 3)

4.2.1.2   Reactor model 2

Reactor model 2 handles the most types of feedstocks, in particular two types of naphta and 5 light gases, expecting the highest uncertainties in prediction performance. As figure 4-4 shows, the highest deviations can be observed for the components ethylene, ethane and propylene, which make up the main part of the cracking gas. The neural network performs much better than the polynomial fit, as expected.
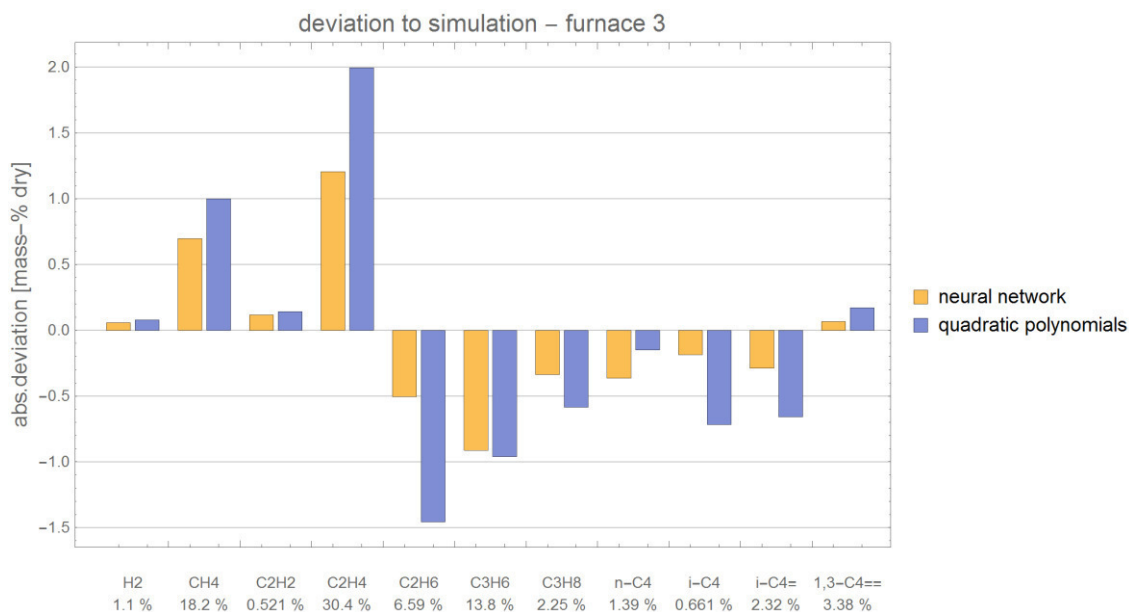
Figure 4-4: abs. deviation to simulation - furnace 3 (case 3)

4.2.1.3   Reactor model 3

Reactor model 3 handles 8 types of feedstocks, in particular these are the same as those for model 2 without ethane.

Figure 4-5: abs. deviation to simulation - furnace 4 (case 3)

This results, as shown in figure 4-5, in a really good prediction performance of the neural network, with a maximum deviation of 0.3%. In contrast, the polynomial fit's prediction performance is much worse.

4.2.1.4   Reactor model 4

Reactor model 4 utilizes only light gases, from ethane to C4-mixes as feed. There-fore, a slightly lower prediction performance is expected.
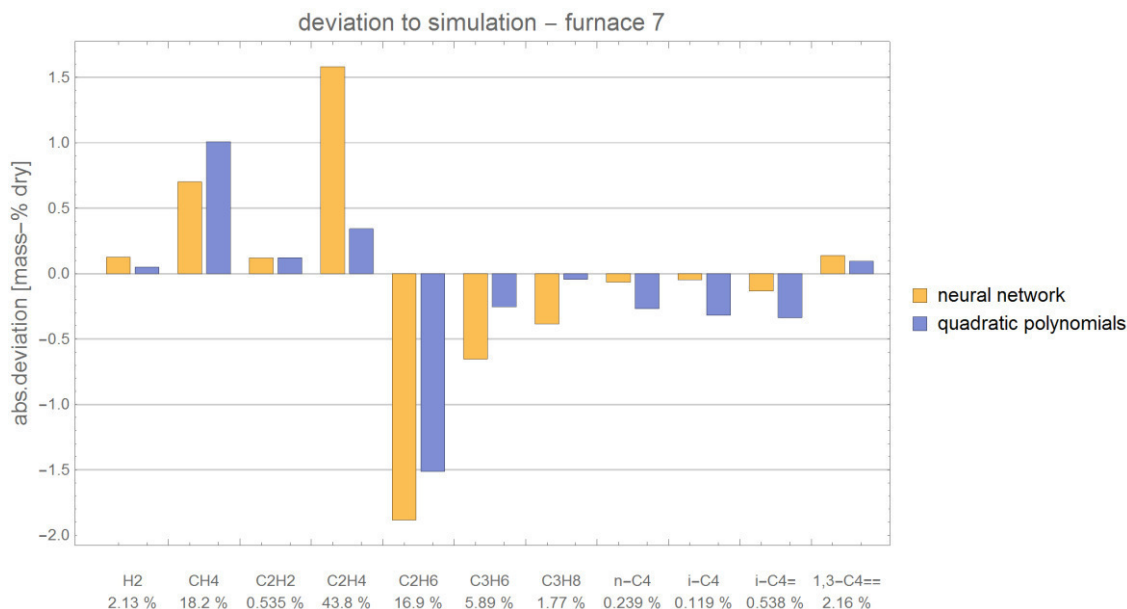
Figure 4-6: abs. deviation to simulation - furnace 7 (case 3)

The result, as shown in figure 4-6, is even worse, the neural network's deviation for ethylene and ethane is higher than the polynomial fit's one. It ranges from +1.51% to –1.8%.

4.2.1.5   Reactor model 5

Reactor model 5 handles only ethane as feedstock, resulting in only 3 prediction pa-rameters, so a good prediction performance is expected. In this case, the neural net-work's prediction performance for ethylene and ethane is quite bad. As figure 4-7 shows, the ethylene's mass fraction is 1.5% too high and the ethane's one 2.2% too low.

There are many attempts made to improve the performance, from shrinking and heavily expanding the network topology to excessive training. None of these really improved the performance, it is supposed that the size of generated training data should be expanded, which is apparently (with 240 data points) too small.
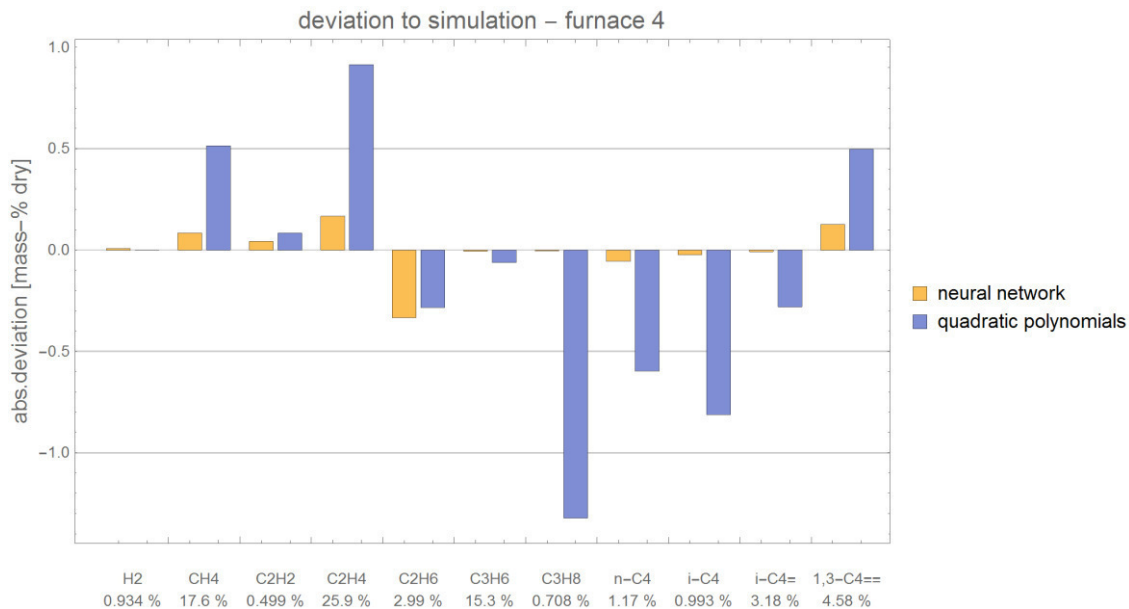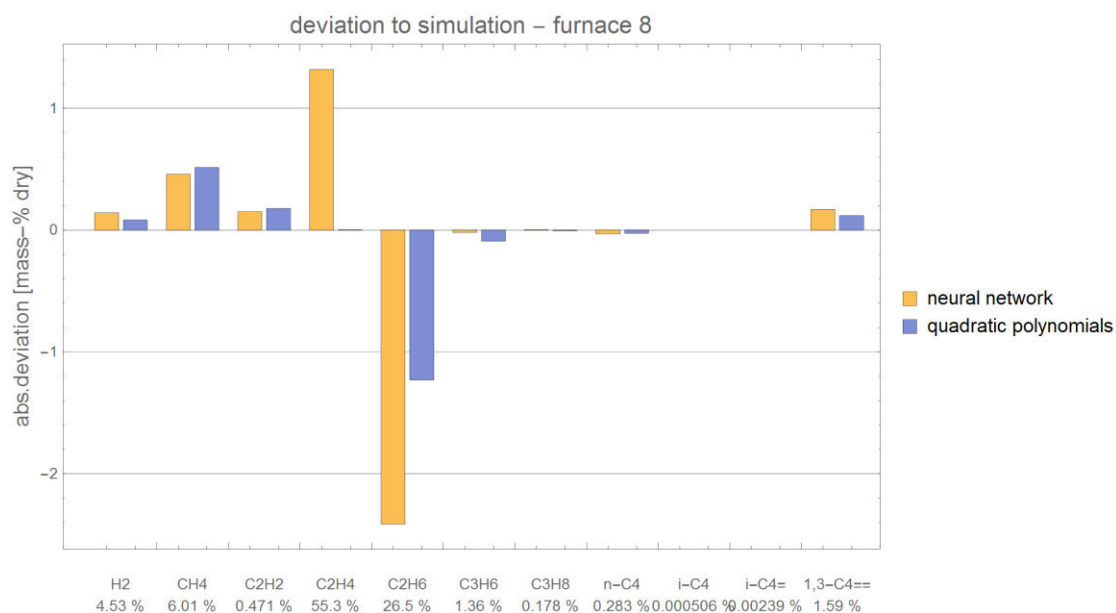
Figure 4-7: abs. deviation to simulation - furnace 8 (case 3)

4.2.1.6 Reactor model 6

Reactor model calculates the cracking of one naphta feed. As shown in figure 4-8, the neural network and the polynomial fit perform nearly equally, the neural network's performance for ethylene is slightly better, but also shows a deviation of nearly 0.6%. To further improve the model, a larger training set is necessary.
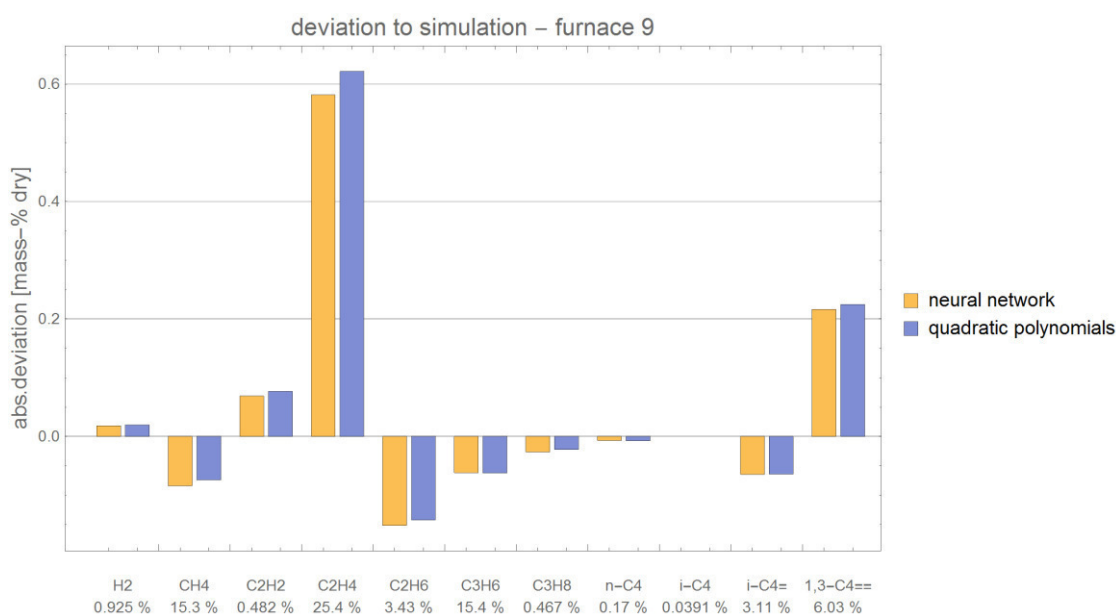
Figure 4-8: abs. deviation to simulation - furnace 9 (case 3)

4.2.2   Plant products

The quite strong deviations of the key components ethylene and ethane with the same trend, for both model types, will of course affect the overall plant product streams. Therefore, the plant products are calculated by a shortcut method, where the plant is considered as a component splitter. The calculation of the light gases is trivial, whereby the LPG stream consists of the C4 fraction without iso-Butene and Butadiene. The light pyrolysis gas (PyGas Light) includes components ranging from C5 to C6 (without Benzene), while the heavy pyrolysis gas components (PyGas Heavy) range from C7 to C10. All heavier components are considered as gas oil.
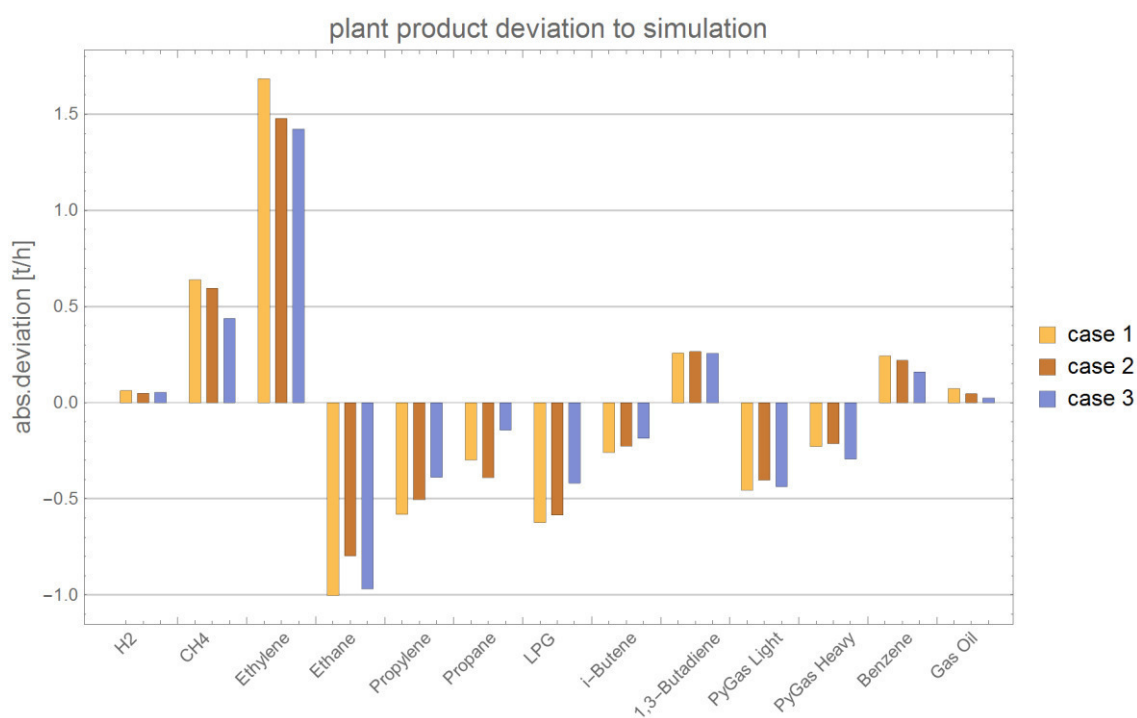
Figure 4-9: plant product deviation to simulation - absolute

This is done for all three validation cases, the resulting absolute deviations are shown in figure 4-9 and the relative deviations are shown in figure 4-10.

It can be clearly seen, that each component stream's deviation tends to the same direction. Validation case 3 shows for all components the smallest deviation. Even though the absolute deviation for the key products hydrogen, methane, ethylene, propylene and butadiene is very different, the relative deviation (2-3%) is nearly the same. Thereby, the by-products ethane, propane and LPG show a strong trend to be

underestimated by the models, the relative deviations in a range of -5 to -12% are quite high, while their absolute deviation in a range of -0.5 to 1 t/h is quite low.
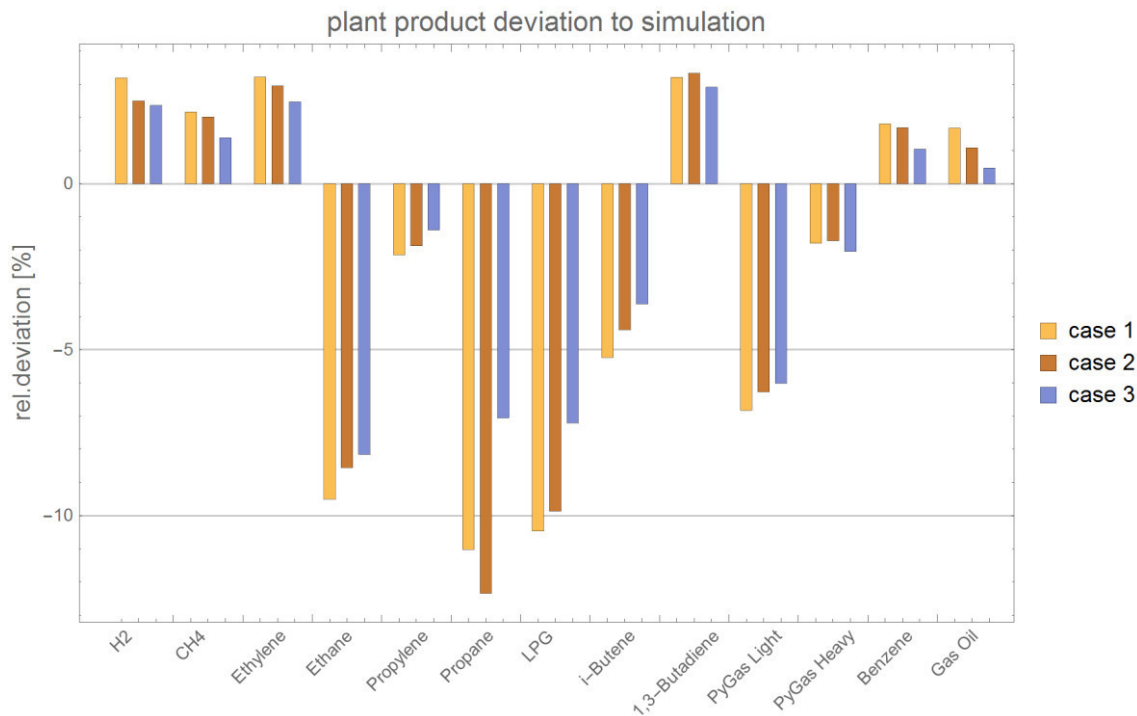
Figure 4-10: plant product deviation to simulation - relative

4.3   Comparison to measurements

Finally, the calculated cracked gas compositions are compared to measured data. Therefore, absolute deviations of the simulated data and both models to measurement data for each furnace are calculated. To point out the trend in prediction precision, the furnaces are grouped by their feed types. In the following figures, the numbers below the component names denote the measured dry mass fraction values of the component.

4.3.1.1   Naphta cracking

Furnaces no. 1, 9 and 10 are fed with pure naphtha. Looking at the absolute deviations in figure 4-11, figure 4-12 and figure 4-13 leads to the conclusion, that the reaction kinetic simulation is very accurate, the worst case can be found for ethylene with a deviation of -2.6% for furnaces 9 and 10. The high i-Butene deviation in figure 4-12 is an outlier, due to the fact that the measured value is zero and the deviation for that component at furnace 10, which is operating with the same feed and parameters as furnace 9, is nearly zero.
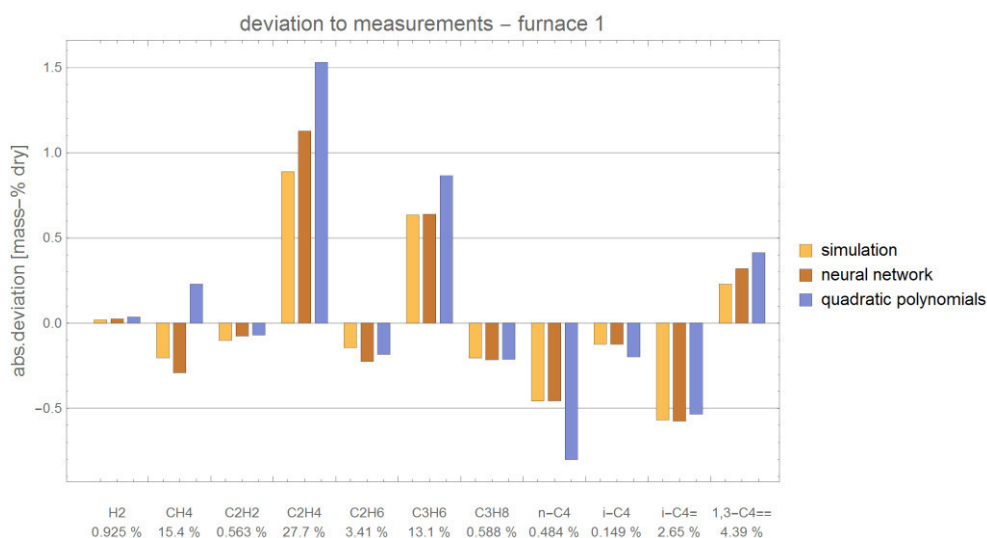
Figure 4-11: abs. deviation to measurements - furnace 1 (case 3)
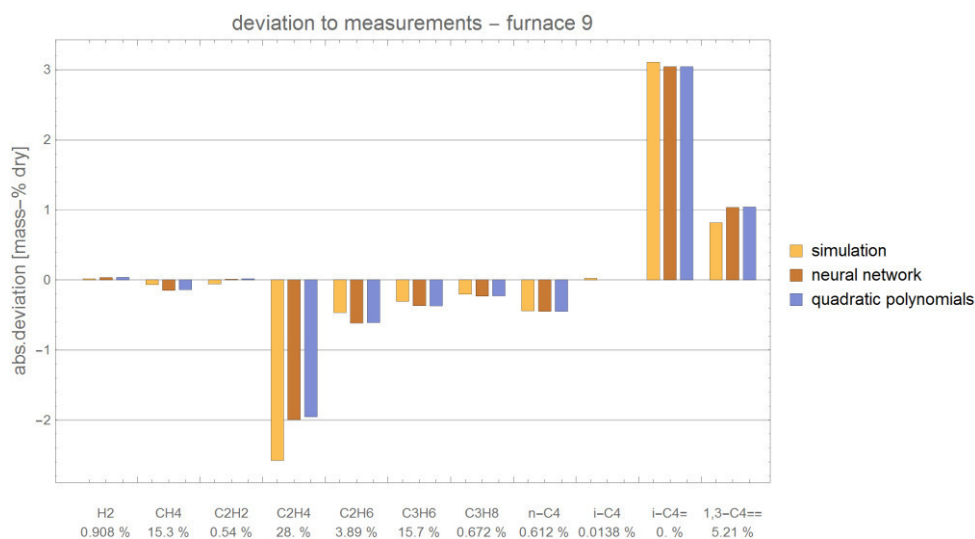
Figure 4-12: abs. deviation to measurements - furnace 9 (case 3)
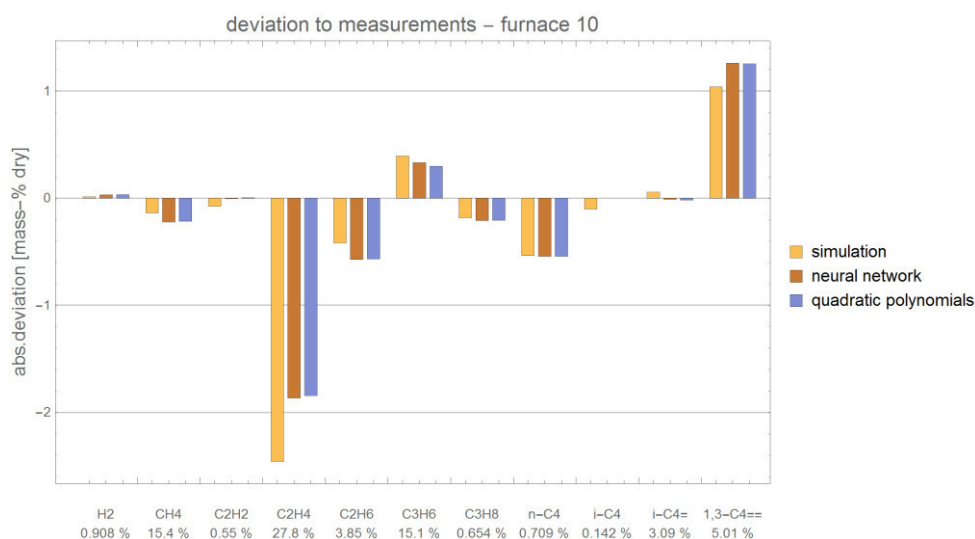
Figure 4-13: abs. deviation to measurements - furnace 10 (case 3)

4.3.1.2   Co-cracking

Furnaces 3 to 6 are in co-cracking operation mode, thus the feeds are composed of naphtas mixed with light gases, ranging from C2 to C4. Due to the uncertainties in determining the co-crack composition from process data of the feedstock management system, bigger deviations are expected. Figure 4-14 to figure 4-17 show the results for these furnaces, the simulation deviations for ethylene lie in a range from 2% to 4%. Also the deviations for i-Butene are quite high with more than -2%.
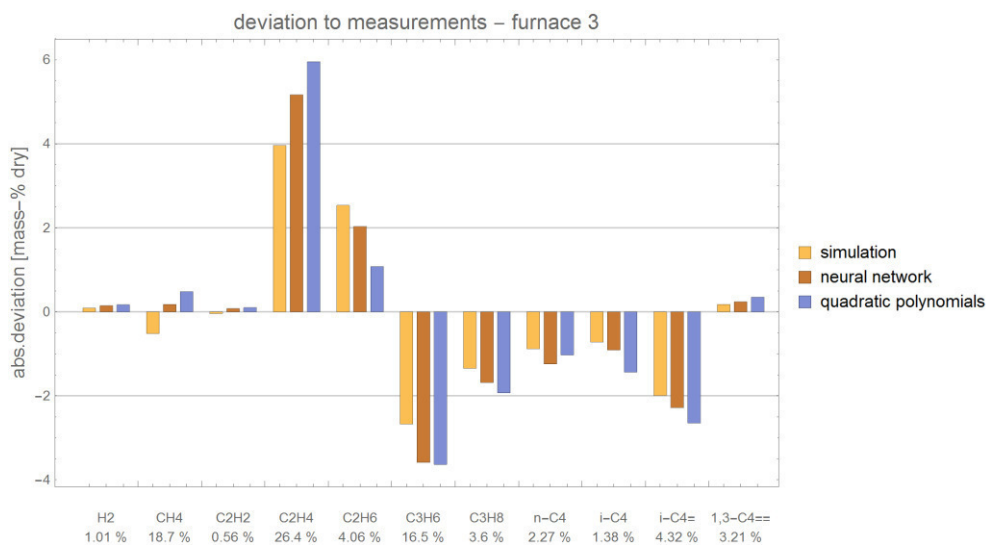
Figure 4-14: abs. deviation to measurements - furnace 3 (case 3)
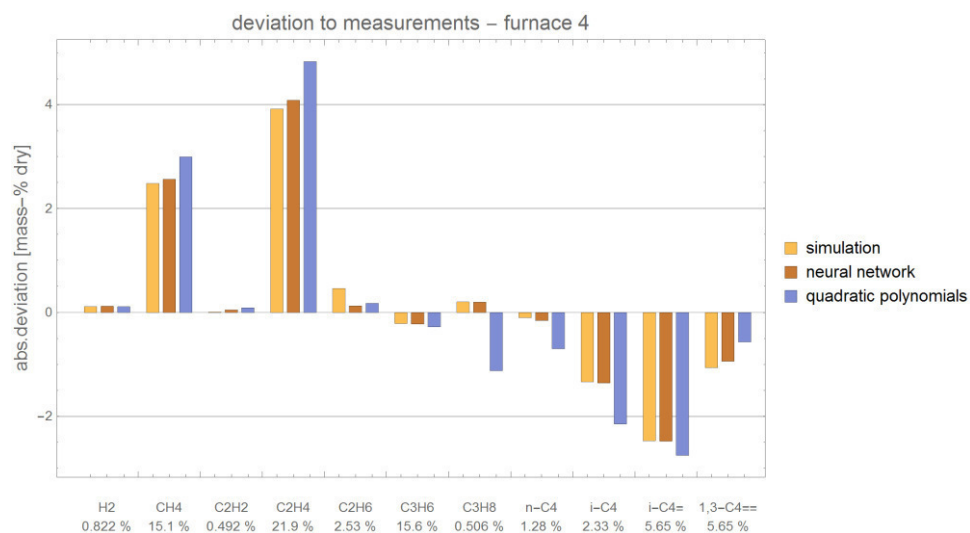
Figure 4-15: abs. deviation to measurements - furnace 4 (case 3)
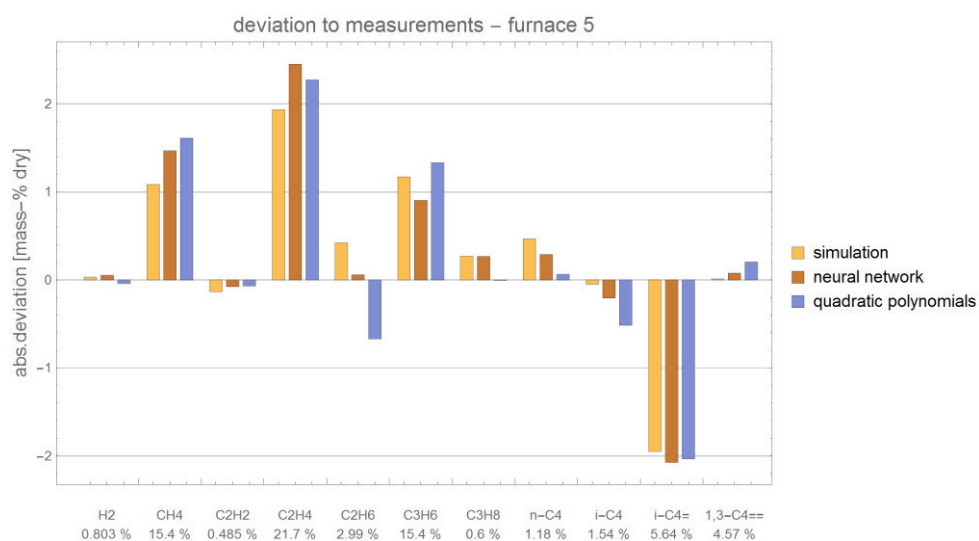
Figure 4-16: abs. deviation to measurements - furnace 5 (case 3)
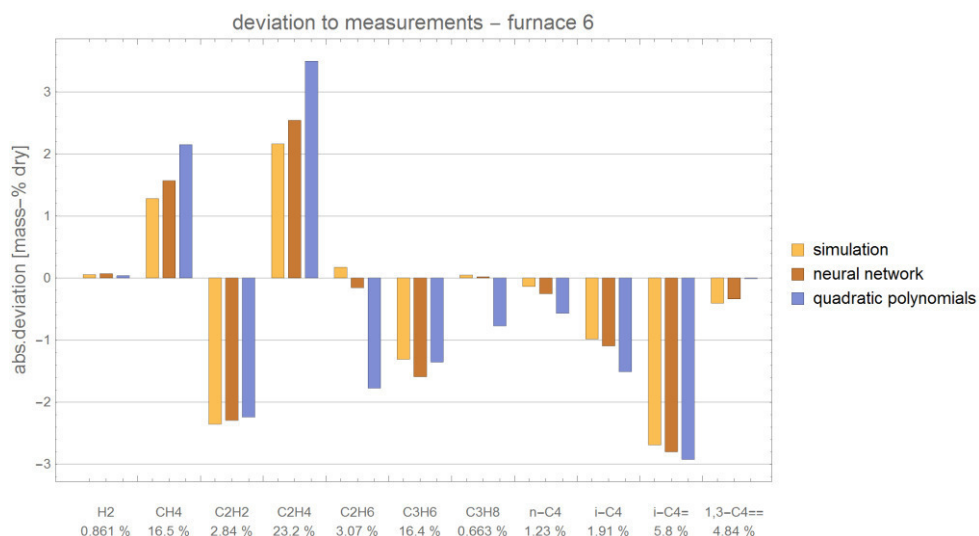
Figure 4-17: abs. deviation to measurements - furnace 6 (case 3)

4.3.1.3   Gaseous feedstocks

Furnaces 7 and 8 are operated with gaseous feedstocks, no. 7 with mixes ranging from C2 to C4, no. 8 with pure ethane. As already stated, the prediction performance
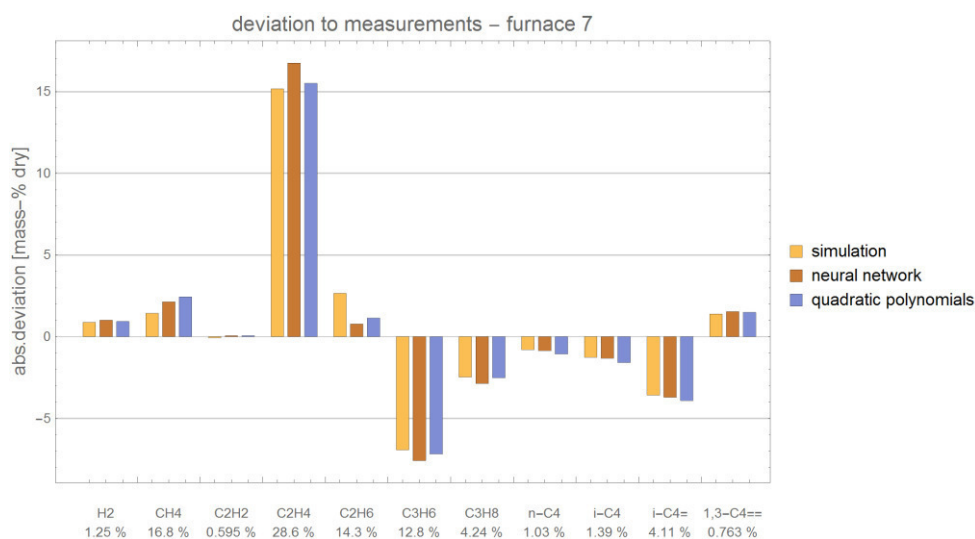
Figure 4-18: abs. deviation to measurements - furnace 7 (case 3)

is expected to be limited for no.7 due to the uncertainties in the feed composition. As figure 4-18 shows, the simulation is far away from the measured values, especially the ethylene value is 15% too high.

The simulation of furnace 8 is expected to perform better, due to the single ethane feedstock. Figure 4-19 points out, that deviations are quite high here as well, espe-

cially ethylene and ethane are about 4% too high or too low. It is also obvious, that the neural network performs poor for this furnace.
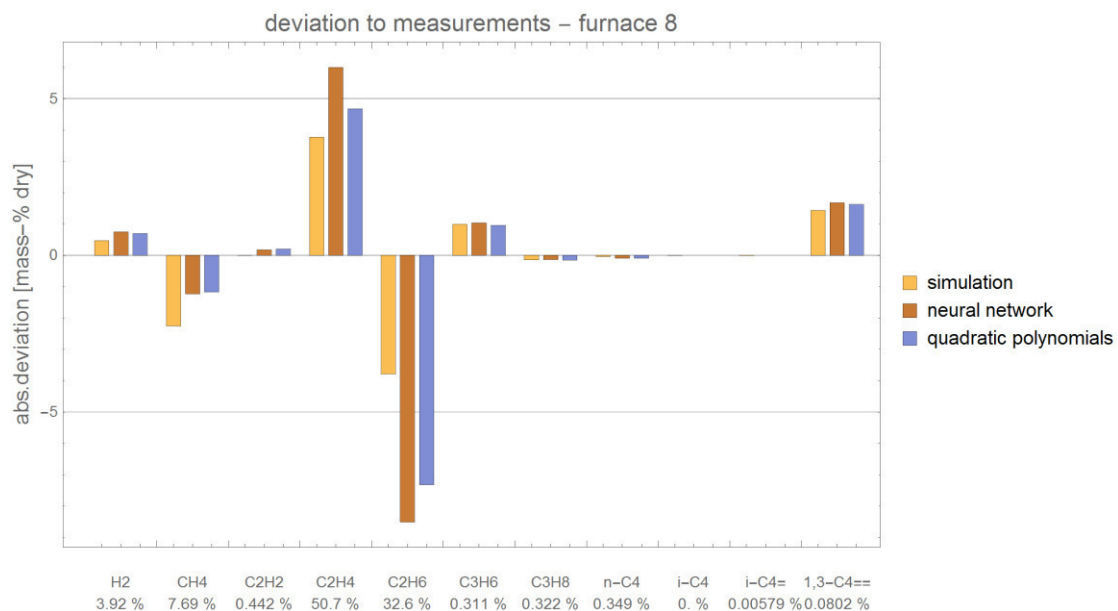
Figure 4-19: abs. deviation to measurements - furnace 8 (case 1)

4.4   Modeling effort vs. prediction performance

Finally, both modeling methods have to be evaluated. To measure the model development effort, the computation time for model development is compared with the example of reactor 2, which is the most extensive one, involving 21180 simulation cases.

Both model types base on the same datasets, whose generation by simulation consumes the biggest part of the time, but runs automatically. Generation of 21180 cases by Mathematica takes about 3 hours, while running all simulations lasts about 4 days. Transferring this data from one PC to another takes another 2 hours. The data import into Mathematica, calculating to dray mass fractions and exporting the dataset takes about 15 minutes time. The only difference can be found in the network training time and time spent on function fitting. While function fitting takes 5 seconds, the network training with 120000 rounds lasts 3 hours and 14 minutes. The postprocessing, in particular the packaging of the functions and the network as well as the transformation parameters only takes seconds.

Therefore, the really time consuming part for developing such a black box model is the handling and running of the kinetic simulations, while function fitting and network training make up only a small part of it.

The prediction performance of neural network models, as expected, is for naphtha and co-cracking operation significantly better than the polynomial models. Nevertheless, the performance of the neural networks for the gaseous feedstock cracking is even worse than the quadratic polynomials, the reason for that can be found in a too little number of simulation data. Increasing the number of simulation cases would lead to a better performance in training and therefore in prediction.

5   Conclusion and outlook

Developing black-box models for steam cracking furnaces is a task of facing problems in a wide area of simulation and programming, from coupling the radical kinetic simulation program by XML-files with Excel and Mathematica, over data importing and exporting issues to neural network design and training. The most time consuming part is the generation of data by radical kinetic simulation, which takes all in all about two weeks for all 6 reactor models.

Artificial neural models are a good choice for building up black box models of complex and very sensitive systems like steam crackers, but their ability to predict the reactor effluent composition is not perfect. The resulting neural models perform very good for naphta cracking, while the prediction performance decreases significantly when gaseous feedstocks are cracked or co-cracked with naphta. It seems, that the number of training data was too small for the neural network models showing larger deviations to simulation data. Therefore, it would be necessary to choose a smaller step size between the input parameters of the simulations, resulting in a larger number of simulation cases.

Nevertheless, the ability to calculate the mass fractions of 35 to 77 components out of an input involving only 5 to 9 parameters is outstanding, while the computational time of the network is nearly zero. If a further refinement for the reactor models processing gaseous feedstocks is done, these black-box models are ready to be utilized for plant-wide optimization.

The reactor models consisting of fitted quadratic polynomials also showed a good performance in view of their simplicity. These models are supposed to be used for integration of a simplified ethylene plant in a refinery-wide LP-tool.

Naturally, the precision of the developed models can never overcome the precision of the radical kinetic simulation, which showed weaknesses in case of cracking gaseous feedstocks. The reason for that can be found in the poor measurements of the feed management system of the specific streams, so further improvements have to start at this point.

Due to the flexibility of neural networks, they can be used as a universal tool for developing data driven models for industry 4.0 applications, where the mechanisms inside the systems are not well known or unknown. Examples for future applications range from modelling reactors processing distillation residues over reactor catalyst deactivation to heat exchanger fouling.

6 Appendix

6.1 Fitted functions

Table 6-1: coefficients of polynomial reactor model 1

Component	Intercept	Naphta 2	Naphta 2²	Naphta 3	Naphta 3²	Naphta 4	Naphta 4²	COT	COT²	STR	STR²
Hydrogen	-0,04548	-3,5E-05	-2,7E-07	-6,9E-05	1,93E-07	-7,7E-05	3,63E-07	9,15E-05	-2,9E-08	0,000902	-0,00066
Methane	-1,11552	-0,00027	-1,8E-05	-0,00204	9,74E-06	-0,00224	1,4E-05	0,00256	-1,1E-06	-0,07886	0,02873
Acetylene	0,223264	7,49E-06	-5,6E-07	-2,9E-05	1,61E-07	-3,7E-05	2,83E-07	-0,0006	4,06E-07	0,003592	-0,00119
Ethylene	-3,3892	-0,00031	-1,5E-05	-0,00143	4,42E-06	-0,00187	1,53E-05	0,007985	-4,3E-06	0,058325	-0,04542
Ethane	-0,60925	-0,0001	3,71E-07	-0,00021	1,12E-06	-0,00012	2,02E-07	0,001679	-1,1E-06	-0,05363	0,027357
Propadiene	-0,01655	5,59E-05	-8,8E-07	-7,9E-06	1,69E-07	-5,3E-05	8,34E-07	-1,2E-05	4,61E-08	0,00524	-0,00227
Propylene	-4,36166	0,001922	-1,5E-05	0,000521	2,75E-06	-0,0001	1,27E-05	0,011494	-7,3E-06	0,049464	-0,03277
Propane	-0,09619	3,25E-06	4,13E-07	1,79E-05	2,64E-08	3,01E-05	-3,6E-08	0,000274	-1,8E-07	-0,00601	0,003143
n-Butane	0,497456	0,001184	-1E-05	-0,00016	1,93E-06	-0,00012	1,39E-06	-0,00108	5,76E-07	0,00877	-0,00193
i-C4	0,101245	0,000238	-2E-06	-2,2E-05	3,26E-07	-1,9E-05	1,99E-07	-0,00022	1,13E-07	0,001395	-0,00019
i-C4=	-0,57634	0,000844	-6,9E-06	0,00024	1,07E-06	-9,3E-05	4,22E-06	0,001674	-1,2E-06	0,013234	-0,00746
1-C4=	0,155478	0,000377	-8,7E-08	0,000408	-9,7E-08	0,00035	6,41E-07	-0,00017	-2,1E-08	0,015655	-0,00472
2-C4=	-0,00923	0,00033	-2,1E-06	8,52E-05	3,46E-07	6,04E-05	5,64E-07	0,000129	-1,4E-07	0,006181	-0,00304
1,3-C4==	-1,2959	7,35E-06	7,27E-07	0,000321	-2,6E-07	0,000347	1,11E-06	0,003198	-1,9E-06	0,034388	-0,01966
Benzene	-0,53228	-0,00251	1,95E-05	0,000519	-1,8E-05	-0,0009	-2,2E-06	0,001119	-4E-07	-0,05319	0,020365
Toluene	-0,53848	-0,00159	1,72E-05	-0,00012	-1,8E-06	0,000856	-1,4E-05	0,001379	-8E-07	-0,02264	0,009467
Xylene	-0,08067	-0,00049	6,94E-06	-0,00023	1,76E-06	0,000822	-7,2E-06	0,000275	-2E-07	-0,00059	0,000397
Ethylbenzene	-0,02687	-2,7E-05	2,56E-07	-5,9E-06	-6,4E-08	1,06E-05	-1,7E-07	6,77E-05	-4,1E-08	-0,00075	0,000392
Styrene	0,320638	-0,0004	2,88E-06	-8,1E-05	-2,2E-06	-0,00012	-1,2E-06	-0,00086	5,92E-07	-0,01026	0,004511
C9 Aromatics	0,048151	-5,9E-05	1,03E-06	-2,3E-05	4,86E-08	0,000145	-3,3E-07	-9,2E-05	4,18E-08	0,000236	0,000143
n-C5	1,223107	0,001374	-9,6E-06	-3,5E-05	2,27E-07	-1,7E-05	-3,4E-07	-0,00282	1,61E-06	0,012133	-0,00144
i-C5	1,164388	0,001286	-9,3E-06	-4E-05	3,9E-07	-1,6E-05	-4,5E-07	-0,00269	1,53E-06	0,0108	-0,00129
n-C6	1,474991	0,000267	9,82E-07	0,00073	1,24E-06	4,54E-05	-2,1E-06	-0,00345	2E-06	0,011572	-0,00047
n-C7	0,837562	-4,4E-05	1,76E-06	0,000234	2,2E-07	0,000266	2,31E-07	-0,00198	1,16E-06	0,005463	0,000252
n-C8	0,372544	-7,9E-06	5,45E-07	3,06E-05	-5,6E-07	0,00016	8,3E-07	-0,00088	5,21E-07	0,002007	0,000326
n-C9	0,141572	2,02E-07	1,42E-07	1,09E-05	-2,5E-07	5,34E-05	3,66E-07	-0,00034	2E-07	0,000629	0,000202
Cyclo-C5	0,121227	8,06E-05	-3,7E-07	3,92E-05	2,06E-09	-6,1E-07	-7,7E-08	-0,00028	1,62E-07	0,001296	-0,00011
Methylcyclo-C5	0,367045	4,13E-05	4,52E-07	0,000209	5,87E-07	1,55E-05	-5,5E-07	-0,00086	5,01E-07	0,003182	4,66E-06
C7 Naphthene	0,582388	-1,4E-05	9,05E-07	0,000157	3,02E-07	0,000168	1,83E-07	-0,00138	8,12E-07	0,003477	0,000529
C8 Naphthene	0,524909	3,09E-06	4,8E-07	7,58E-05	-3,4E-07	0,000159	8,51E-07	-0,00125	7,43E-07	0,00224	0,000806
C9 Naphthene	0,062085	1,27E-06	3,88E-08	5,5E-06	-1,1E-07	2E-05	1,73E-07	-0,00015	8,86E-08	0,00022	0,000126
2-M-C4=	0,127673	4,65E-05	-1,8E-07	2,49E-05	2,13E-08	1,43E-05	-7,9E-08	-0,0003	1,74E-07	0,000819	-0,00017
1-C5=	0,350483	3,97E-05	2E-07	7,72E-05	-4,1E-08	7,63E-05	2,35E-07	-0,00082	4,8E-07	0,001495	-6,7E-05
Naphthalene	-0,02211	-0,00069	7,68E-06	-7,8E-05	-2,7E-06	-9,4E-05	-2,9E-06	-1,7E-05	9,22E-08	-0,0169	0,007096
1-M-C4=	0,099552	0,000116	-3,9E-07	7,44E-05	7,88E-08	4,62E-05	8,13E-08	-0,0002	9,78E-08	0,002722	-0,00053
Dimethylcyclo-C6	0,081464	-6,6E-07	7,57E-08	8,6E-06	-4,2E-08	1,88E-05	9,04E-08	-0,00019	1,12E-07	5,02E-05	4E-05
i-C10	0,023409	5,1E-07	1,37E-08	2,05E-06	-4,3E-08	7,26E-06	6,63E-08	-5,6E-05	3,34E-08	7,85E-05	4,78E-05
C5==	0,010177	1,33E-05	3,32E-07	6,97E-05	-2,5E-08	9,68E-05	4,3E-07	4,05E-06	-1,8E-08	0,00387	-0,0018
Isoprene	-0,08193	1,14E-05	1,01E-06	0,000153	-2E-07	0,000193	3,26E-08	0,00027	-2,1E-07	0,006206	-0,00268
i-C6=	0,064004	3,09E-05	-1,1E-07	2,11E-05	4,35E-09	4,57E-06	-2,4E-08	-0,00015	8,27E-08	0,000498	-7,6E-05
Methylcyclo-C6	0,12743	-9,6E-06	2,08E-07	1,79E-05	-8,8E-08	3,5E-05	1,88E-07	-0,00029	1,7E-07	-4,1E-05	0,000128
i-C6	1,526937	0,000572	-1,9E-06	0,000377	3,54E-07	8,12E-05	-2,1E-06	-0,0036	2,11E-06	0,009282	0,000218

1,3-C6==	0,058121	4,03E-06	4,65E-08	1,25E-05	1,92E-09	1,42E-05	7,09E-08	-0,00014	7,82E-08	0,000243	-4,8E-05
1,3-M-C5==	-0,00458	1,21E-05	1,86E-07	6,06E-05	2,52E-08	6,96E-05	2,74E-07	4,45E-05	-4,6E-08	0,002182	-0,00097
C7 Aromatics	0,15814	1,5E-06	1,39E-07	3,11E-05	1,09E-07	3,69E-05	8,68E-08	-0,00038	2,24E-07	0,000582	0,000201
M-Cylco-C5=	0,10955	1,06E-05	3,25E-08	2,35E-05	1,25E-08	1,98E-05	6,52E-08	-0,00025	1,44E-07	0,000133	-7,4E-05
i-C7	1,073748	-3,4E-05	1,81E-06	0,000333	1,03E-06	0,000228	-3,1E-07	-0,00255	1,5E-06	0,005764	0,00063
M-C6==	0,101238	2,54E-05	-4,4E-08	3,22E-05	2,24E-08	2,89E-05	2,31E-07	-0,00023	1,24E-07	0,000891	-0,0003
Cylco-C5==	-0,90642	-0,00014	2,43E-06	0,00017	-6,2E-07	0,000174	4,73E-08	0,002321	-1,5E-06	0,005703	-0,00463
C8 Aromatics	0,055251	6,02E-08	5,46E-08	4,76E-06	-7,9E-08	1,91E-05	1,39E-07	-0,00013	7,81E-08	0,000248	3,93E-05
Cylco-C5=	-0,03778	-3,7E-06	2,81E-07	3,95E-05	-1,5E-08	2,22E-05	1,96E-08	0,000134	-1E-07	-0,00036	-0,00038
i-C8	0,419002	-4,2E-06	5,11E-07	4,51E-05	-4,8E-07	0,00015	8,69E-07	-0,001	5,9E-07	0,001954	0,00044
i-C9	0,259062	2,03E-06	2,23E-07	2,09E-05	-4,5E-07	8,93E-05	7,04E-07	-0,00062	3,68E-07	0,00103	0,0004
Cyclo-C6=	0,063147	-1,1E-05	1,54E-07	1,14E-05	-2,3E-08	1,76E-05	8,81E-08	-0,00014	8,15E-08	-0,00014	9,49E-05
C4H4	0,044194	-2,4E-06	-1,2E-07	-7,8E-06	2,9E-08	-8,9E-06	4,72E-08	-0,00012	7,72E-08	0,000401	-0,00023
M-Styrene	-0,06125	-0,00024	2,81E-06	-6,6E-05	-7,4E-08	0,000106	-2,3E-06	0,000143	-7,2E-08	-0,00455	0,001923
Dimethylstyrene	-0,03251	-5,1E-05	7,1E-07	-1,6E-05	7,45E-08	3,97E-05	-5,8E-07	8,16E-05	-4,9E-08	-0,00074	0,000279
C16H18 Aromatics	0,009387	-1,8E-05	2,49E-07	-2,2E-06	-9,6E-09	2,71E-05	-1,2E-07	-1,8E-05	9,11E-09	-0,00028	0,000154
C16H12 Aromatics	0,211709	-0,00076	7,54E-06	-0,00026	-4,1E-07	0,00024	-7,9E-06	-0,00059	4,37E-07	-0,01779	0,008606
M-Cylco-C5==	-0,03642	7,95E-06	2,82E-07	7,97E-05	-4,7E-08	8,31E-05	2,16E-07	0,000146	-1,2E-07	0,002198	-0,0013
M-Cyclo-C6==	0,032152	-7E-06	1,25E-07	6,96E-06	-3,1E-08	8,62E-06	1,45E-08	-6,9E-05	3,66E-08	-0,00031	4,41E-05
Indene	-0,08232	-0,00021	2,49E-06	-3,8E-05	-3E-07	4,74E-05	-1,8E-06	0,000198	-1,1E-07	-0,00515	0,002302
C22 Aromatics	0,060634	-0,00013	1,42E-06	-5,7E-05	9,76E-08	3,61E-05	-1,4E-06	-0,00016	1,12E-07	-0,00339	0,001683
C7==	0,040693	4,91E-06	3,22E-08	1,09E-05	-9,2E-09	8,39E-06	1,48E-08	-9,1E-05	5,09E-08	0,000128	-0,00011
C32H26 Aromatics	0,013796	-3E-05	3,63E-07	-1,6E-05	7,32E-08	1,46E-05	-3,5E-07	-3,6E-05	2,44E-08	-0,00092	0,000493
C40 Aromatics	0,033065	-7E-05	7,28E-07	-4,5E-05	3,27E-07	4,18E-05	-1,1E-06	-8,7E-05	6,01E-08	-0,00211	0,001153
C32H20 Aromatics	0,535945	-0,00063	5,57E-06	-0,00031	3,08E-07	7,19E-05	-7,7E-06	-0,0014	9,46E-07	-0,02296	0,012672
C42 Aromatics	0,178026	-0,00011	7,23E-07	-8,1E-05	5,19E-07	1,81E-05	-1,8E-06	-0,00046	2,97E-07	-0,00448	0,002619
2-C5=	0,179193	7,46E-05	-2E-07	5,58E-05	7,67E-09	3,61E-05	-2,5E-08	-0,00041	2,29E-07	0,001781	-0,00045
1-C6=	0,168629	4,82E-06	1,96E-07	3,84E-05	-9,8E-08	4,37E-05	2,85E-07	-0,0004	2,34E-07	0,00091	-1,8E-05
2-M-C5=	0,094296	-3,3E-06	1,68E-07	2,54E-05	1,97E-08	2,33E-05	2,88E-08	-0,00022	1,31E-07	0,000495	-4E-05
1-C8=	0,023031	-2,3E-07	2,86E-08	1,82E-06	-3,9E-08	9,33E-06	5,98E-08	-5,5E-05	3,24E-08	0,00012	1,2E-05
1-M-C4=	0,117974	3,88E-05	-1,3E-08	3,8E-05	-1,1E-08	3,83E-05	3,16E-08	-0,00027	1,49E-07	0,001182	-0,00031
C6==	0,048514	-3,9E-07	5,51E-08	9,12E-06	1E-08	9,51E-06	3,17E-08	-0,00012	6,9E-08	0,000168	7,97E-06
1-M-C5=	0,081954	1,59E-07	7,31E-08	1,25E-05	-2,7E-09	1,5E-05	8,7E-08	-0,0002	1,17E-07	0,000213	3,3E-05
1-C7=	0,067471	-1,9E-06	1,05E-07	9,49E-06	-7,8E-08	2,42E-05	1,58E-07	-0,00016	9,44E-08	0,000374	-6,3E-06
CO	0,051571	-2,1E-05	-1,5E-07	-2,8E-05	2,79E-08	-3E-05	6,78E-08	-0,00015	1,05E-07	0,003221	-0,00117

Table 6-2: coefficients of polynomial reactor model 2 - 1/2

Component	Intercept	Naphta 2	Naphta 2²	Naphta 3	Naphta 3²	C4-Mix	C4-Mix²	C2	C2²	C3	C3²
Hydrogen	-0,08255	-0,00032	1,86E-06	-0,00038	3,34E-06	-0,00054	1,03E-05	0,000257	2,59E-05	-0,00012	5,75E-07
Methane	-1,9419	-0,0017	3,19E-06	-0,00389	3,37E-05	-0,00081	-4,3E-05	-0,00569	-4,5E-05	-0,00094	-5,7E-06
Acetylene	0,436076	-8,6E-05	2,77E-07	-0,00012	2,11E-07	-4,7E-05	-1,5E-07	-3,5E-05	-1,7E-06	-8,3E-05	-6,3E-07
Ethylene	-5,75377	-0,00261	5,5E-06	-0,00452	4,13E-05	-0,0092	1,42E-05	0,007309	-6,5E-06	-0,00085	-2,2E-05
Ethane	-0,43588	-0,00108	5,33E-06	-0,00104	-3,4E-07	-0,00265	3,54E-05	0,022982	-0,0004	-0,00209	2,61E-05
Propadiene	-0,37341	4,62E-06	6,82E-08	-7,6E-05	6,81E-07	0,000209	-2,7E-06	-0,00044	-2,3E-06	-0,00018	-5,4E-07
Propylene	-5,27055	0,002733	-7,3E-06	0,001366	1,17E-06	0,00442	-6,2E-05	-0,00789	9,17E-05	0,002798	-2,2E-05
Propane	2,467599	-0,00019	-3,1E-06	0,00014	-1,7E-05	-2,2E-05	-1,4E-05	-0,00113	2,14E-05	0,009989	-7,1E-05
n-Butane	3,885036	0,000768	-2,5E-06	0,000423	-1,9E-05	0,000895	-3,2E-06	-0,00064	2,52E-05	-0,00017	9,07E-06
i-C4	4,821595	0,000331	-6,8E-06	0,000571	-2,3E-05	0,001764	1,18E-05	-0,00061	2,6E-05	-1E-04	8,93E-06
i-C4=	-0,74042	0,000476	-9,1E-07	0,000157	-5,7E-06	0,001918	-9,6E-07	-0,00242	5,11E-05	-0,00119	1,09E-05
1-C4=	0,063761	0,000414	8,37E-07	0,000322	4,01E-06	0,000422	-3E-07	-0,00063	1,96E-05	0,000134	2,21E-07
2-C4=	0,767719	0,000315	2,9E-07	0,000224	-1,9E-06	0,000444	2,18E-05	-0,00046	1,85E-05	-4,7E-05	1,39E-06
1,3-C4==	-0,60224	0,000501	-1,5E-06	0,00051	5E-06	0,001031	2,97E-05	-0,0015	2,58E-05	-0,00056	1,04E-06
Benzene	-0,31363	-0,00062	-2,1E-06	0,002235	-2,5E-05	0,000508	1,67E-05	-0,00336	3,6E-05	-0,00266	1,63E-05
Toluene	-0,5124	-0,0002	-1,3E-06	0,000936	-3,2E-06	0,000283	5,32E-06	-0,00157	3,38E-05	-0,00102	1,23E-05
Xylene	-0,15521	-1,6E-05	-2,3E-07	0,000118	4,24E-08	8,75E-05	-5,5E-08	-0,00034	1,05E-05	-0,0002	3,64E-06
Styrene	0,520162	-0,00016	-1,7E-08	0,000241	-6,1E-06	-6,4E-05	-6,2E-08	-0,00026	-4,3E-06	-0,00037	2,29E-06
n-C5	0,597754	0,000556	3,05E-06	5,73E-05	-2,4E-06	5,83E-05	-2,6E-06	-4,9E-05	3,48E-06	1,79E-06	7,63E-07
i-C5	0,634544	0,000498	3,41E-06	6,12E-05	-2,5E-06	7,98E-05	-1,5E-06	-4,7E-05	3,49E-06	3,11E-06	7,72E-07
n-C6	0,601935	0,000131	3,88E-07	0,000242	7,54E-06	5,73E-05	-2,6E-06	-2,9E-05	2,29E-06	8,81E-06	2,65E-07
n-C7	0,133266	4,52E-06	-9,3E-08	5,32E-05	2,28E-06	1,25E-05	-5,4E-07	-3,5E-06	3,56E-07	2,99E-06	6,4E-09
Cyclo-C5	0,052538	3,79E-05	7,53E-08	2,04E-05	2,72E-07	7,24E-06	-3,5E-07	-4,7E-06	2,81E-07	1,82E-08	5,1E-08
Methylcyclo-C5	0,136454	2,57E-05	1,2E-08	7,61E-05	2,07E-06	1,74E-05	-8,4E-07	-6,9E-06	4,9E-07	2,49E-06	3,09E-08
C7 Naphthene	0,083262	2,91E-06	-4,4E-08	3,24E-05	1,39E-06	8,73E-06	-3,7E-07	-1,4E-06	1,86E-07	2,45E-06	-1E-08
C8 Naphthene	0,025225	9,87E-07	-1,4E-08	6,68E-06	3,86E-07	2,4E-06	-9,2E-08	-4,6E-08	4,22E-08	8,76E-07	-5,5E-09
2-M-C4=	0,044899	1,6E-05	1,8E-07	7,92E-06	2,08E-07	4,41E-06	-1,3E-07	-3,2E-06	2,68E-07	7,1E-07	3,48E-08
1-C5=	0,056966	2,41E-05	8,84E-08	1,78E-05	6,71E-07	4,17E-06	-3E-07	6,27E-06	-2,8E-07	6,07E-06	3,17E-08
Naphthalene	-0,00095	-0,00013	-7,3E-07	0,000321	5,93E-08	0,000125	3,64E-07	-0,00056	6,59E-06	-0,00052	6,95E-06
1-M-C4=	0,0555	7,71E-05	1,3E-07	4,28E-05	3,01E-07	9,29E-05	-4,1E-07	-0,00012	4,49E-06	-2,6E-05	4,22E-07
C5==	-0,12837	6,72E-05	7,86E-08	4,51E-05	1,49E-06	7,59E-05	-8,7E-07	-0,00015	1,28E-06	-1,2E-05	-7,4E-09
Isoprene	-0,11204	9,95E-05	1,77E-07	0,000116	2,71E-06	9,75E-05	-1,7E-06	-0,00022	6,75E-06	-7,2E-05	5,18E-07
i-C6	0,521491	0,000168	1,25E-06	0,000114	2,84E-06	4,42E-05	-1,6E-06	-1,6E-05	1,75E-06	1,2E-05	2,39E-07
1,3-M-C5==	-0,11625	3,76E-05	1,2E-08	3,13E-05	1,02E-06	7,63E-05	-1E-06	-0,00017	5,39E-06	-6,1E-05	3,97E-07
M-Cylco-C5=	0,047061	1,23E-05	7,14E-09	1,24E-05	1,46E-07	1,82E-05	1,88E-07	-2,8E-05	1,1E-06	6,08E-07	-2,1E-08
i-C7	0,195436	7,59E-06	-1,5E-07	6,25E-05	3,28E-06	1,68E-05	-6,7E-07	-3,4E-06	4,7E-07	5,12E-06	8,58E-10
M-C6==	0,034836	2,24E-05	-2,3E-08	1,4E-05	1,39E-07	4,44E-05	-1,2E-07	-8,3E-05	3,31E-06	-2,2E-05	3,27E-07
Cylco-C5==	-0,56029	0,000175	-2,8E-07	0,000245	4,35E-06	0,000284	-2,8E-06	-0,00037	5,14E-06	-0,00013	3,74E-07
Cylco-C5=	-0,00864	3,62E-05	8,67E-08	3,21E-05	9,69E-07	2,77E-05	-8E-07	-2E-05	-7,2E-07	-1,1E-05	-1,4E-07
C4H4	0,101452	-2,1E-05	4E-08	-2,2E-05	-5E-08	-5,9E-07	2,02E-07	-1,6E-05	-1,6E-07	-2,7E-05	-9,7E-08
M-Styrene	0,003574	-3,6E-05	-1,4E-07	9,85E-05	-2,6E-07	6,43E-06	5,48E-07	-0,00016	3,02E-06	-0,00013	1,66E-06
C16H12 Aromatics	0,390553	-0,00018	-1,3E-07	0,000377	-6,2E-06	1,16E-05	2,81E-07	-0,00045	3,59E-06	-0,00047	5,73E-06
M-Cylco-C5==	-0,02561	6,38E-05	-2,7E-08	6,61E-05	9,65E-07	0,000113	-5E-09	-0,0002	6,72E-06	-4,5E-05	5,48E-07
Indene	-0,02537	-2,2E-05	-1,8E-07	9,82E-05	1,58E-07	4,25E-05	9,95E-08	-0,00014	2,97E-06	-0,00012	2,26E-06
C22 Aromatics	0,097318	-2,8E-05	-2E-08	4,07E-05	-7,7E-07	-8,7E-06	6,91E-08	-4,7E-05	6,9E-08	-6,3E-05	8,75E-07
C40 Aromatics	0,058797	-1,5E-05	3,82E-08	2,29E-05	-7E-07	-5,8E-06	-1,4E-08	-2,1E-05	1,21E-07	-2,9E-05	3,8E-07
C32H20 Aromatics	0,677932	-0,00021	6,11E-07	0,000327	-9,8E-06	-4,5E-05	-1,5E-07	-0,00032	1,53E-06	-0,0004	5,04E-06

C42 Aromatics	0,206865	-4,3E-05	2,27E-07	4,75E-05	-2,5E-06	-2,6E-05	-3,7E-08	-2,8E-05	-4,8E-07	-6,5E-05	6,93E-07
2-C5=	0,094258	4,35E-05	2,5E-07	2,49E-05	6,5E-07	1,51E-05	-4,1E-07	-8,6E-06	4,75E-07	3,82E-07	1,29E-07
1-C6=	0,025302	5,04E-06	2,45E-09	9,94E-06	3,42E-07	3,45E-06	-1,1E-07	-3,2E-06	2,38E-07	6,62E-07	2,31E-09
1-M-C4=	0,068892	2,68E-05	1,31E-07	1,95E-05	3,17E-07	2,17E-05	1,62E-07	-1,4E-05	7,28E-07	2,92E-06	6,27E-08
CO	0,088798	-4,2E-05	9,53E-08	-4,4E-05	-9,7E-08	-1,3E-05	-2,9E-07	-5,6E-05	-1,3E-07	-5,9E-05	4,41E-08
CO2	0,03724	-1,8E-05	6,58E-08	-1,8E-05	-1,4E-08	-5E-06	-1,7E-07	-1,5E-05	-2,2E-07	-1,9E-05	3,41E-09

Table 6-3: coefficients of polynomial reactor model 2 - 2/2

Component	n-C4	n-C4²	i-C4	i-C4²	COT	COT²	STR	STR²
Hydrogen	-0,00024	-1,7E-06	-0,00021	1,89E-06	0,000157	-4,6E-08	-0,0001	-0,00066
Methane	-0,00095	-4,3E-06	0,000551	-2,4E-05	0,004175	-1,8E-06	-0,08961	0,031257
Acetylene	-7,5E-05	-1,6E-07	-7,9E-05	-7,9E-07	-0,00113	7,41E-07	0,004501	-0,00224
Ethylene	0,001269	-4,2E-05	-0,01168	3,99E-05	0,012929	-6,7E-06	-0,00459	-0,02275
Ethane	-0,0014	2,02E-05	-0,00234	4,42E-06	0,001914	-1,6E-06	0,003181	0,006439
Propadiene	-0,00018	1,04E-06	0,000572	-4E-07	0,000838	-4,6E-07	0,006685	-0,00351
Propylene	0,002661	5,13E-06	0,004916	-2,6E-05	0,013785	-8,8E-06	0,060683	-0,03072
Propane	-0,00066	1,9E-05	-0,0004	2,35E-06	-0,00537	2,89E-06	0,025638	-0,00413
n-Butane	0,005368	-5,8E-05	-8,3E-05	4,21E-06	-0,00887	5,03E-06	0,022191	-0,00148
i-C4	-0,00024	1,55E-05	0,004707	-1,5E-05	-0,01107	6,32E-06	0,022882	-0,00041
i-C4=	-0,00129	1,82E-05	0,005952	9,29E-06	0,002267	-1,6E-06	0,02382	-0,01022
1-C4=	0,000295	4,7E-07	0,000295	-2,3E-06	-5E-05	-3E-08	0,007096	-0,00145
2-C4=	0,000137	8,34E-07	5,65E-05	-2,1E-06	-0,00175	9,9E-07	0,004683	-0,00053
1,3-C4==	-9,3E-05	3,23E-06	-0,00044	-9,2E-06	0,001437	-8,2E-07	0,017078	-0,00989
Benzene	-0,00192	2,56E-06	-0,00111	2,44E-06	0,000478	-4E-10	-0,04632	0,017511
Toluene	-0,00072	3,94E-06	-1,3E-05	-4,9E-06	0,001198	-6,6E-07	-0,01812	0,007306
Xylene	-0,00015	1,73E-06	6,08E-05	-6,8E-07	0,000374	-2,2E-07	-0,00303	0,001144
Styrene	-0,00025	-1,1E-06	-0,00038	5,51E-06	-0,00133	8,59E-07	-0,00944	0,004446
n-C5	-1,7E-05	1,93E-06	8,42E-06	3,26E-07	-0,00139	8,02E-07	0,002164	0,000208
i-C5	-1,2E-05	1,74E-06	1,03E-05	3,08E-07	-0,00148	8,55E-07	0,002043	0,00024
n-C6	-1,2E-05	1,61E-06	1,07E-05	1,36E-07	-0,00141	8,2E-07	0,001639	0,00043
n-C7	-1,7E-06	3,12E-07	2,88E-06	1,17E-08	-0,00031	1,83E-07	0,000273	0,000142
Cyclo-C5	-2,8E-06	2,36E-07	1,68E-07	3,32E-08	-0,00012	7,02E-08	0,000233	2,57E-05
Methylcyclo-C5	-5E-06	5,14E-07	2,29E-06	3,93E-08	-0,00032	1,85E-07	0,000481	0,000123
C7 Naphthene	-9,6E-07	2,11E-07	2,16E-06	6,29E-09	-0,0002	1,15E-07	0,000158	0,000118
C8 Naphthene	9,2E-09	5,06E-08	7,8E-07	1,33E-10	-6E-05	3,51E-08	2,48E-05	4,69E-05
2-M-C4=	2,68E-07	6,56E-08	1,4E-06	-3,2E-09	-0,00011	6,17E-08	9,3E-05	2,29E-05
1-C5=	1,25E-05	9,16E-08	-5,6E-06	3,84E-08	-0,00013	7,27E-08	-6,7E-05	9,28E-05
Naphthalene	-0,00036	2,28E-06	-0,00035	3,46E-06	-5,9E-05	9,36E-08	-0,01001	0,004136
1-M-C4=	-2,1E-05	2,97E-07	0,000225	2,23E-06	-0,0001	4,42E-08	0,001377	-0,00026
C5==	2,87E-05	3,65E-07	4,9E-05	-2,5E-06	0,000311	-1,9E-07	0,001348	-0,00087
Isoprene	-5,5E-05	2,46E-07	0,000221	-4,2E-07	0,000296	-1,9E-07	0,001542	-0,0007
i-C6	-1,2E-06	1,08E-06	1,39E-05	1,08E-07	-0,00123	7,18E-07	0,001028	0,000489
1,3-M-C5==	-4,4E-05	-7,8E-08	0,000219	-2,8E-06	0,000298	-1,9E-07	0,000581	-0,00047
M-Cylco-C5=	5,37E-06	1,4E-08	1,12E-05	-8,9E-08	-0,00011	5,99E-08	3,25E-05	-3,9E-05
i-C7	-6,8E-07	3,76E-07	5,02E-06	4,68E-09	-0,00046	2,71E-07	0,000309	0,000237
M-C6==	-1,4E-05	6,13E-08	0,00011	4,62E-07	-6,8E-05	3,19E-08	0,000446	-0,00023
Cylco-C5==	3,47E-06	-7,3E-08	3,91E-06	8,1E-07	0,001402	-8,7E-07	0,002049	-0,00201

Component								
Cylco-C5=	2,42E-05	-8,5E-08	-7,4E-05	1,34E-06	3,87E-05	-3,1E-08	-0,00075	0,000135
C4H4	-2,1E-05	-5,4E-08	-3,6E-05	1,41E-08	-0,00026	1,63E-07	0,00034	-0,0003
M-Styrene	-8,5E-05	1,58E-07	-4,2E-05	-4,5E-07	-2,1E-05	2,55E-08	-0,00305	0,001444
C16H12 Aromatics	-0,00035	1,15E-06	-0,00032	4,28E-06	-0,00101	6,66E-07	-0,01231	0,006138
M-Cylco-C5==	-1,5E-05	7,15E-08	0,000171	-1,3E-06	9,25E-05	-7,3E-08	0,001044	-0,00063
Indene	-8,2E-05	8,8E-07	-7,3E-05	1,02E-06	5,57E-05	-2,6E-08	-0,00267	0,001259
C22 Aromatics	-4,3E-05	4,11E-09	-6,1E-05	1,25E-06	-0,00024	1,55E-07	-0,00194	0,001053
C40 Aromatics	-2,1E-05	3,04E-09	-2,8E-05	6E-07	-0,00015	9,22E-08	-0,00109	0,000639
C32H20 Aromatics	-0,00032	1,45E-06	-0,00033	4,22E-06	-0,0017	1,08E-06	-0,01343	0,007519
C42 Aromatics	-4,9E-05	-3,7E-08	-8E-05	1,98E-06	-0,00051	3,18E-07	-0,00267	0,001631
2-C5=	2,7E-06	1,97E-07	-6,6E-07	6,43E-08	-0,00022	1,27E-07	0,000227	3,31E-05
1-C6=	5,07E-07	5,2E-08	9,91E-08	5,19E-08	-5,9E-05	3,39E-08	4,06E-05	2,35E-05
1-M-C4=	6,2E-06	7,51E-08	5,94E-06	-1,1E-07	-0,00016	9,13E-08	0,000241	-5E-06
CO	-3,6E-05	-1,5E-07	-4,7E-05	7,84E-09	-0,00024	1,66E-07	0,004288	-0,00168
CO2	-1,5E-05	-2,5E-08	-1,7E-05	9,64E-09	-9,6E-05	6,23E-08	0,000969	-0,00029

Table 6-4: coefficients of polynomial reactor model 3 - 1/2

Component	Intercept	Naphta 2	Naphta 2²	Naphta 3	Naphta 3²	C4-Mix	C4-Mix²	C3	C3²
Hydrogen	-0,10351	-9,4E-05	-9E-08	-0,00014	6,83E-07	-0,00026	4,52E-06	2,89E-06	2,82E-06
Methane	-1,98211	-0,0026	4,74E-06	-0,00465	3,23E-05	-0,00213	-2,5E-05	-0,00203	-2,7E-06
Acetylene	0,324926	-4,4E-05	2,53E-07	-7,4E-05	3,4E-07	-1,8E-06	-2,9E-07	-3E-05	-1E-06
Ethylene	-4,0772	0,000548	-1,7E-05	-0,00099	6,23E-06	-0,00638	8,26E-06	0,001339	-1,4E-05
Ethane	-0,71893	0,000311	-1,4E-06	8,76E-05	3,37E-06	-0,00107	2,17E-05	-0,00035	8,01E-06
Propadiene	-0,15547	-7E-05	8,13E-07	-0,00015	1,86E-06	0,000122	-1,8E-06	-0,00021	-2,2E-06
Propylene	-6,41129	0,001094	1,65E-06	-0,00033	1,3E-05	0,002574	-4,8E-05	0,001368	-3,2E-05
Propane	2,099399	-0,00072	9,01E-06	-0,00029	-9,9E-06	-0,0004	-9,7E-06	0,01208	-8,7E-05
n-Butane	3,769122	0,000709	2,49E-06	0,000217	-1,4E-05	0,000967	-1,7E-06	-0,0004	1,23E-05
i-C4	4,732871	5,85E-05	2,17E-06	0,000394	-2E-05	0,002238	1,1E-05	-0,00032	1,22E-05
i-C4=	-1,49418	-8E-05	4,91E-06	-0,00046	2,14E-06	0,001578	-5,3E-06	-0,0019	1,49E-05
1-C4=	0,135982	0,000432	-4,1E-07	0,00037	2,33E-06	0,000409	3,5E-06	6,73E-06	2,03E-06
2-C4=	0,995512	0,000328	-2,4E-07	0,00021	-2,4E-06	0,000679	2,69E-05	-0,00016	3,6E-06
1,3-C4==	-0,8239	0,000383	-1,5E-06	0,000519	1,96E-06	0,001257	2,44E-05	-0,00079	2,75E-06
Benzene	-0,22521	-0,00132	5,32E-08	0,001492	-1,8E-05	-0,00028	1,27E-05	-0,00332	1,66E-05
Toluene	-0,44988	-0,00057	4,04E-07	0,000677	-5,4E-06	-7E-05	3,54E-06	-0,00146	1,72E-05
Xylene	-0,14626	-8,8E-05	7,4E-08	7,78E-05	-1,1E-06	3,23E-05	-1,1E-06	-0,00031	5,46E-06
Styrene	0,433577	-0,00019	-3,5E-07	0,000118	-2,5E-06	-0,00014	1,83E-07	-0,00038	7,13E-07
n-C5	0,788059	0,000894	-2,1E-06	6,13E-05	-2,3E-06	6,8E-05	-2,5E-06	-1,6E-05	2E-06
i-C5	0,825556	0,000809	-1,2E-06	6,55E-05	-2,6E-06	0,000102	-1,3E-06	-1,7E-05	2,05E-06
n-C6	0,842533	0,000224	-3,3E-07	0,000448	5,82E-06	8,67E-05	-3,2E-06	1,03E-05	8,2E-07
n-C7	0,202309	4,41E-06	1,03E-07	0,000116	1,94E-06	2,25E-05	-8E-07	6,36E-06	4,71E-08
Cyclo-C5	0,071924	5,98E-05	-2,4E-07	3,14E-05	1,59E-07	1,01E-05	-3,8E-07	-1,9E-07	1,18E-07
Methylcyclo-C5	0,196353	4,22E-05	-2,3E-08	0,000137	1,49E-06	2,87E-05	-1,1E-06	6,1E-06	8,05E-08
C7 Naphthene	0,134199	3,65E-06	9,92E-08	7,39E-05	1,19E-06	1,75E-05	-5,9E-07	6,35E-06	-1,3E-08
C8 Naphthene	0,047686	1,7E-06	2,78E-08	1,95E-05	3,88E-07	5,86E-06	-1,8E-07	2,65E-06	-1,1E-08
2-M-C4=	0,065547	2,95E-05	2,23E-08	1,56E-05	1,67E-07	6,2E-06	-1,5E-07	-5,7E-07	1,44E-07
1-C5=	0,083252	3,62E-05	-6E-08	3,52E-05	6,56E-07	4,36E-06	-2,7E-07	4,16E-06	1,25E-07
Naphthalene	0,072396	-0,00027	-3,5E-07	0,00018	-2,6E-07	-1,7E-05	-5,8E-07	-0,00066	7,98E-06

1-M-C4=	-0,00641	8,45E-05	-1,2E-07	4,09E-05	4,33E-07	8,53E-05	-6,2E-07	-6,2E-05	1,23E-06
C5==	-0,10788	4,88E-05	-1,6E-07	4,93E-05	8,66E-07	4,69E-05	-2,4E-07	-4,9E-05	1,74E-07
Isoprene	-0,15905	8,69E-05	-2,3E-07	0,00014	1,42E-06	5,73E-05	-1,4E-06	-0,00013	1,38E-06
i-C6=	0,045956	2,29E-05	-4,2E-08	1,54E-05	1,25E-07	6,04E-06	-1,5E-07	5,25E-08	4,27E-08
Methylcyclo-C6	0,013867	2,7E-06	-1,3E-08	9,68E-06	1,86E-07	1,1E-05	1,55E-07	-1,5E-05	6,39E-08
i-C6	0,792851	0,000328	-4,4E-07	0,00022	2,2E-06	7,32E-05	-2,2E-06	1,72E-05	8,58E-07
1,3-M-C5==	-0,15086	1,32E-05	3E-08	2,3E-05	7,72E-07	4,84E-05	-1,1E-06	-0,00011	9,74E-07
C7 Aromatics	0,02889	9,94E-07	8,68E-09	1,05E-05	2,22E-07	4,41E-06	-7,9E-08	-5,8E-07	3,69E-08
M-Cylco-C5=	0,066739	1,37E-05	-1,9E-08	1,72E-05	1,08E-07	2,61E-05	2,06E-07	-6,8E-06	1,05E-07
i-C7	0,317231	9,36E-06	9,24E-08	0,000151	3,06E-06	3,27E-05	-1,1E-06	1,13E-05	6,54E-08
M-C6==	-0,00468	1,47E-05	8,28E-09	7,28E-06	2,91E-07	4,15E-05	-3,5E-07	-5,2E-05	9,2E-07
Cylco-C5==	-0,65303	9,37E-05	-6,4E-07	0,000228	2,7E-06	0,000214	-3E-06	-0,00026	1,05E-06
Cylco-C5=	-0,00804	4,38E-05	-1,2E-07	4,99E-05	6,92E-07	3,36E-05	-1E-06	-1,9E-05	-2,3E-07
i-C8	0,021198	7,16E-07	8,42E-09	8,87E-06	1,87E-07	2,35E-06	-7,2E-08	9,87E-07	-5,2E-10
Cyclo-C6=	-0,00167	1,97E-06	-4E-08	7,58E-06	1,75E-07	8,69E-06	-2,5E-07	-1,1E-05	-6,7E-08
C4H4	0,072792	-1,4E-05	5,87E-08	-1,6E-05	2,59E-08	8,73E-06	9,68E-08	-1,7E-05	-2,1E-07
M-Styrene	0,022579	-7,2E-05	-7,8E-08	6,25E-05	-3,7E-07	-3,6E-05	4,15E-07	-0,00017	2,06E-06
C16H12 Aromatics	0,36856	-0,00028	1,3E-07	0,000226	-4,5E-06	-0,00011	-4,4E-08	-0,00055	5,48E-06
M-Cylco-C5==	-0,08771	3,77E-05	-8,6E-08	6,26E-05	6,21E-07	0,000102	1,55E-09	-0,00011	1,81E-06
M-Cyclo-C6==	0,017734	4,22E-06	-4,1E-08	7,32E-06	1,13E-07	8,08E-06	3,13E-07	-1,2E-05	1,89E-07
Indene	-0,01974	-5,6E-05	-1,2E-07	7,05E-05	-3,8E-07	1,37E-05	-4,5E-07	-0,00016	2,98E-06
C22 Aromatics	0,079355	-3,6E-05	-4,8E-08	2,16E-05	-4,3E-07	-2,1E-05	7,41E-08	-6,9E-05	7,86E-07
C40 Aromatics	0,043053	-1,8E-05	1,15E-08	1,15E-05	-3,9E-07	-1,1E-05	-1,3E-08	-3E-05	2,81E-07
C32H20 Aromatics	0,550839	-0,00026	6,17E-07	0,000172	-6,3E-06	-0,00013	-2,6E-07	-0,00043	3,98E-06
C42 Aromatics	0,136768	-3,9E-05	6,19E-08	1,98E-05	-1,2E-06	-3E-05	-3,4E-09	-5,3E-05	1,66E-07
2-C5=	0,118822	6,77E-05	-1,7E-07	4,27E-05	4,4E-07	1,9E-05	-4,8E-07	-5,8E-06	3,92E-07
1-C6=	0,033312	7,38E-06	-1,2E-08	1,84E-05	2,85E-07	5,16E-06	-1,7E-07	5E-07	2,18E-08
2-M-C5=	0,030157	1,11E-06	5,18E-10	1,1E-05	2,42E-07	3,96E-06	-7,2E-08	5,85E-07	-1E-08
1-M-C4=	0,088284	3,9E-05	-5,5E-08	3,05E-05	2,22E-07	3,21E-05	1,11E-07	-1,3E-06	2,51E-07
CO	0,069374	-4E-05	8,81E-08	-4,3E-05	3,05E-08	-1,3E-05	-2,6E-07	-5,6E-05	-3,1E-08
CO2	0,02829	-1,9E-05	6,9E-08	-1,9E-05	4,3E-08	-8,2E-06	-1,3E-07	-1,9E-05	-5,1E-08

Table 6-5: coefficients of polynomial reactor model 3 - 2/2

Component	n-C4	n-C4²	i-C4	i-C4²	COT	COT²	STR	STR²
Hydrogen	-8E-05	-3,1E-07	5,11E-06	3,09E-07	0,000224	-1E-07	0,00076	-0,00083
Methane	-0,00188	-6,6E-06	-0,00084	-4,5E-06	0,004438	-2,1E-06	-0,10062	0,033732
Acetylene	-2,7E-05	-5,4E-07	-2,9E-05	-8,6E-07	-0,00087	5,76E-07	0,004676	-0,00186
Ethylene	0,00341	-1,4E-05	-0,00854	9,33E-06	0,009195	-4,7E-06	0,019346	-0,03034
Ethane	0,000379	-5,3E-07	-0,00071	-3E-06	0,001827	-1,1E-06	-0,03158	0,016597
Propadiene	-0,00021	-4,6E-07	0,000438	7,38E-07	0,000297	-1,2E-07	0,007501	-0,00362
Propylene	0,0015	-7,5E-06	0,002766	-1,8E-06	0,016636	-1,1E-05	0,06032	-0,03639
Propane	-0,0011	2,29E-05	-0,00088	1,08E-05	-0,0045	2,36E-06	0,030308	-0,0049
n-Butane	0,007237	-8,6E-05	-0,00039	1,22E-05	-0,00859	4,84E-06	0,031396	-0,00299
i-C4	-0,00057	2,39E-05	0,006489	-4,2E-05	-0,01086	6,18E-06	0,032646	-0,00168
i-C4=	-0,00202	2,31E-05	0,00627	-1,6E-05	0,004123	-2,8E-06	0,024011	-0,01255
1-C4=	0,000227	1,35E-06	0,000119	1,58E-06	-0,0002	5,09E-08	0,009335	-0,00159
2-C4=	5,17E-05	3,11E-06	-6,7E-05	7,1E-07	-0,00228	1,29E-06	0,007833	-0,00103

1,3-C4==	-0,00032	5,32E-06	-0,00076	-1,5E-06	0,001999	-1,2E-06	0,02616	-0,01399
Benzene	-0,00257	9,19E-07	-0,00192	7,21E-06	0,000278	1,4E-07	-0,05534	0,020356
Toluene	-0,00113	6,94E-06	-0,0004	-3,3E-06	0,00106	-5,7E-07	-0,02589	0,010718
Xylene	-0,00025	2,97E-06	-1,5E-05	-3,9E-07	0,000355	-2,1E-07	-0,00488	0,001912
Styrene	-0,00027	-2,2E-06	-0,00041	4,85E-06	-0,00112	7,41E-07	-0,0094	0,004264
n-C5	-5,4E-05	4,09E-06	-1,8E-05	2,13E-06	-0,00184	1,06E-06	0,004069	0,000247
i-C5	-5E-05	3,86E-06	-1,7E-05	2,05E-06	-0,00193	1,12E-06	0,003849	0,000265
n-C6	-3,2E-05	3,17E-06	2,72E-06	1,21E-06	-0,00198	1,16E-06	0,003393	0,000667
n-C7	-3,8E-06	6,06E-07	3,98E-06	1,67E-07	-0,00048	2,82E-07	0,000637	0,000253
Cyclo-C5	-5,6E-06	4,2E-07	-1,4E-06	1,8E-07	-0,00017	9,7E-08	0,00044	4,23E-05
Methylcyclo-C5	-8,2E-06	8,76E-07	2,5E-06	2,76E-07	-0,00046	2,69E-07	0,000957	0,000231
C7 Naphthene	-1,2E-06	4E-07	4,32E-06	9,1E-08	-0,00032	1,87E-07	0,000385	0,000238
C8 Naphthene	3,78E-07	1,13E-07	2,01E-06	2,04E-08	-0,00011	6,74E-08	8,12E-05	0,00011
2-M-C4=	-1,4E-06	1,96E-07	1,98E-08	1,16E-07	-0,00015	9,09E-08	0,000212	1,15E-05
1-C5=	1,18E-05	2,32E-07	-1,2E-05	3,52E-07	-0,00019	1,1E-07	1,59E-05	0,000129
Naphthalene	-0,0005	3,04E-06	-0,0005	5,41E-06	-0,00024	2,1E-07	-0,01297	0,005411
1-M-C4=	-5,2E-05	8,5E-07	0,000249	7,7E-07	4,94E-05	-5E-08	0,001779	-0,00036
C5==	-8,6E-07	3,54E-07	-1,5E-05	-8,8E-07	0,000264	-1,6E-07	0,001609	-0,00103
Isoprene	-0,00011	9,64E-07	0,000182	-5,3E-07	0,000414	-2,7E-07	0,00192	-0,00098
i-C6=	1,81E-06	-3,1E-08	1,64E-05	-5,2E-07	-0,00011	6,08E-08	0,000111	3,22E-05
Methylcyclo-C6	-7,3E-06	-7,1E-09	-4,7E-06	-1,3E-07	-2,7E-05	1,25E-08	-0,00026	4,35E-05
i-C6	-1,3E-05	2,51E-06	1,24E-05	1,08E-06	-0,00188	1,1E-06	0,002378	0,000838
1,3-M-C5==	-8,4E-05	2,37E-07	0,000209	-3,9E-06	0,000385	-2,4E-07	0,000395	-0,00052
C7 Aromatics	-1,1E-06	7,53E-08	5,55E-06	2,44E-08	-6,8E-05	4E-08	2,82E-05	5,42E-05
M-Cylco-C5=	1,78E-06	6,84E-08	6,72E-06	-3,8E-08	-0,00015	8,59E-08	4,23E-05	-7,1E-05
i-C7	-2,2E-06	8,04E-07	8,24E-06	2,14E-07	-0,00075	4,45E-07	0,000797	0,000448
M-C6==	-3,7E-05	3,79E-07	0,000132	-8E-07	3,06E-05	-2,9E-08	0,000461	-0,00031
Cylco-C5==	-0,00011	2,87E-07	-0,00016	3,69E-06	0,001639	-1E-06	0,002357	-0,00294
Cylco-C5=	2,11E-05	-1,2E-07	-0,00011	2,47E-06	4,13E-05	-3,5E-08	-0,00058	-6,2E-05
i-C8	6,71E-08	4,95E-08	7,52E-07	1,09E-08	-5E-05	2,99E-08	4,18E-05	3,96E-05
Cyclo-C6=	-2,5E-06	-8,7E-08	-2,6E-05	4,83E-07	8,37E-06	-6,9E-09	-0,00029	5,84E-05
C4H4	-1,2E-05	-1,3E-07	-2,5E-05	-2,1E-07	-0,00019	1,23E-07	0,000537	-0,00036
M-Styrene	-0,00013	3,7E-07	-8,9E-05	1,69E-07	-6,8E-05	5,64E-08	-0,004	0,001916
C16H12 Aromatics	-0,00043	9,21E-07	-0,00041	4,44E-06	-0,00096	6,44E-07	-0,01466	0,007399
M-Cylco-C5==	-6,8E-05	6,96E-07	0,000153	-2,3E-06	0,00025	-1,7E-07	0,00107	-0,00092
M-Cyclo-C6==	-4,6E-06	7,54E-08	-1E-05	5,81E-07	-3,8E-05	2E-08	-0,00015	1,65E-05
Indene	-0,00012	1,4E-06	-0,00012	1,84E-06	4,31E-05	-1,7E-08	-0,0037	0,00175
C22 Aromatics	-5E-05	-3E-08	-6,9E-05	1,18E-06	-0,0002	1,31E-07	-0,00217	0,001189
C40 Aromatics	-2,2E-05	-5,8E-08	-2,8E-05	4,15E-07	-0,00011	6,98E-08	-0,00118	0,000694
C32H20 Aromatics	-0,00035	5,36E-07	-0,00036	2,9E-06	-0,0014	9,05E-07	-0,01511	0,008587
C42 Aromatics	-4E-05	-4E-07	-6,5E-05	1,04E-06	-0,00034	2,17E-07	-0,00247	0,001515
2-C5=	-2,6E-06	4,38E-07	-9,6E-06	4,99E-07	-0,00028	1,6E-07	0,000467	-1,6E-05
1-C6=	-1,4E-07	1,05E-07	-3,9E-07	9,34E-08	-7,8E-05	4,5E-08	9,4E-05	3,49E-05
2-M-C5=	-8,6E-07	7,49E-08	3,22E-06	1,92E-08	-7,1E-05	4,19E-08	5,1E-05	2,13E-05
1-M-C4=	2,56E-06	2,64E-07	1,4E-06	1,1E-07	-0,0002	1,18E-07	0,000431	-3E-05
CO	-3,4E-05	-2E-07	-4,2E-05	-1,3E-07	-0,0002	1,37E-07	0,004069	-0,00155
CO2	-1,5E-05	-7,1E-08	-1,6E-05	-4,2E-08	-7,4E-05	4,9E-08	0,000929	-0,00036

Table 6-6: coefficients of polynomial reactor model 4

	Intercept	C4-Mix	C4-Mix²	C3	C3²	n-C4	n-C4²	i-C4	i-C4²	COT	COT²	STR	STR²
Hydrogen	-0,11366	-0,00095	2,21E-05	0,000303	4,56E-05	-0,00027	-3,3E-06	-0,0006	1,16E-05	0,000226	-7,9E-08	0,000911	-0,00118
Methane	-2,96425	-0,00034	-7,1E-05	-0,00518	-0,00017	-0,00046	6,34E-06	0,002064	-6,9E-05	0,006605	-3,3E-06	-0,08433	0,027428
Acetylene	0,521404	-5,9E-05	-9,9E-07	3,49E-05	-4,2E-06	-7,3E-05	9,41E-09	-6,8E-05	-1,5E-06	-0,00135	8,81E-07	0,00733	-0,00297
Ethylene	-10,2179	-0,01037	1,92E-05	0,013184	-0,00018	-0,00082	3,99E-06	-0,01345	2,59E-05	0,023676	-1,3E-05	0,026257	-0,03758
Ethane	2,253086	-0,00169	3,85E-05	0,01868	-0,00046	-0,00124	2,54E-05	-0,00128	-2E-05	-0,00414	1,79E-06	0,00763	0,009695
Propadiene	-0,70569	0,000358	-3,8E-06	-0,00071	1,54E-05	-5,1E-05	-3,4E-06	0,000745	9,67E-06	0,001665	-9,8E-07	0,008794	-0,00328
Propylene	-0,50775	0,004991	-5,6E-05	-0,00891	0,000263	0,003823	-2,3E-05	0,006441	-3,1E-05	0,002524	-2,2E-06	0,064517	-0,02262
Propane	3,479096	0,000661	-3,9E-05	-0,00132	6,09E-05	0,005059	3,01E-06	0,00041	-2,7E-05	-0,00781	4,35E-06	0,0167	-0,00011
n-Butane	3,404839	0,000558	-6E-06	-0,00065	4,25E-05	9,63E-05	-2,4E-06	0,000275	-1,2E-05	-0,00784	4,5E-06	0,008102	0,001916
i-C4	4,309004	0,000706	1,09E-05	-0,00061	3,85E-05	0,000162	-3,8E-06	0,001447	2,78E-05	-0,00996	5,74E-06	0,008289	0,002828
i-C4=	1,798805	0,001627	7,51E-06	-0,00286	0,000116	-0,00037	-1,4E-05	0,003791	9,79E-05	-0,00376	1,93E-06	0,022374	-0,00588
1-C4=	0,015652	0,000302	-1,9E-07	-0,00056	2,4E-05	0,000211	-1,9E-06	0,000368	-1,4E-06	3,82E-05	-6,6E-08	0,003995	-0,00047
2-C4=	0,362862	0,000104	1,19E-05	-0,00037	1,83E-05	4,34E-05	-2,2E-06	0,000138	-4,6E-06	-0,00081	4,57E-07	0,001802	4,85E-05
1,3-C4==	-0,77168	0,000415	3,47E-05	-0,00118	3,24E-05	1,43E-05	-8,1E-06	9,91E-05	-2,6E-05	0,001827	-1E-06	0,016338	-0,00892
Benzene	-1,23384	0,001527	6,86E-06	-0,0038	5,26E-05	-0,00246	3,95E-06	-0,00026	-1,2E-06	0,002659	-1,3E-06	-0,04043	0,011404
Toluene	-0,84385	0,00052	1,57E-05	-0,00184	4,9E-05	-0,0008	1,56E-06	0,000396	-1,1E-06	0,001998	-1,1E-06	-0,0128	0,003596
Xylene	-0,20515	7,81E-05	4,37E-06	-0,00042	1,5E-05	-0,00015	7,91E-08	0,000123	3,09E-06	0,000497	-3E-07	-0,00163	0,00029
Styrene	0,595363	0,000202	-1E-05	-0,00028	-1E-05	-0,00048	3,55E-06	-0,00036	1,23E-06	-0,00152	9,9E-07	-0,01237	0,005463
Naphthalene	-0,17195	0,000201	1E-05	-0,00063	7,18E-06	-0,00047	2,82E-06	-0,00016	-2,9E-06	0,000352	-1,5E-07	-0,00866	0,003021
1-M-C4=	0,133695	5,86E-05	2,68E-07	-0,00011	5,49E-06	3,73E-06	-7,1E-07	0,00011	4,56E-06	-0,0003	1,65E-07	0,000686	-6,9E-05
C5==	-0,15546	8,8E-05	-7,9E-07	-0,00015	2,83E-06	5,11E-05	-4,6E-07	0,000122	-3,2E-06	0,00038	-2,3E-07	0,001586	-0,00079
Isoprene	-0,0552	8,29E-05	2,05E-07	-0,00019	7,55E-06	-1,5E-05	-1,3E-06	0,000181	3,91E-06	0,000153	-1E-07	0,001028	-0,00047
1,3-M-C5==	-0,00768	7,15E-05	3,44E-08	-0,00017	7,47E-06	-1,1E-05	-1,3E-06	0,000168	2,26E-06	3,96E-05	-3,6E-08	0,000875	-0,00048
M-C6==	0,087749	2,92E-05	1,57E-07	-7,2E-05	3,75E-06	-6,6E-07	-4,4E-07	5,41E-05	2,48E-06	-0,0002	1,1E-07	0,000363	-0,00013
Cylco-C5==	-0,3117	0,000187	1,12E-06	-0,00029	7,61E-06	3,45E-05	-1,9E-06	0,000157	-7,6E-07	0,0008	-5E-07	0,002077	-0,00148
Cylco-C5=	-0,05049	2,08E-06	-1,1E-07	8,49E-06	-7,6E-07	8,82E-06	-1,2E-07	-3,5E-05	-1,7E-07	0,000135	-8,7E-08	-0,0006	3,66E-05
C4H4	0,166971	-1,1E-05	-6,3E-08	-9,7E-06	-5,6E-07	-3,9E-05	6,59E-09	-6,1E-05	3,79E-08	-0,00042	2,64E-07	0,000814	-0,00059
M-Styrene	-0,08903	5,15E-05	1,84E-06	-0,00021	4,48E-06	-0,00012	4,72E-07	1,3E-05	-1,1E-06	0,000201	-1,1E-07	-0,00276	0,001108
C16H12 Aromatics	0,267586	0,000195	2,73E-06	-0,00055	2,2E-06	-0,00055	4,65E-06	-0,00024	1,51E-06	-0,00072	5,03E-07	-0,01347	0,006013
M-Cylco-C5==	0,076308	7,6E-05	6,11E-07	-0,00017	7,32E-06	8,66E-06	-9,9E-07	0,00013	2,22E-06	-0,00016	7,83E-08	0,000939	-0,00042
Indene	-0,05079	2,77E-05	4,09E-06	-0,00015	2,87E-06	-9,8E-05	7,37E-07	-2,3E-05	-6,3E-07	0,000116	-6,2E-08	-0,00233	0,00099
C22 Aromatics	0,125099	1,84E-05	-6,1E-08	-5,3E-05	-1E-06	-8,4E-05	9,05E-07	-6,4E-05	6,43E-07	-0,00031	1,99E-07	-0,0025	0,001257
C40 Aromatics	0,113972	1,25E-05	-5,7E-07	-2,6E-05	-3,7E-07	-4,9E-05	6,76E-07	-4,1E-05	7,65E-07	-0,00028	1,74E-07	-0,0017	0,000963
C32H20 Aromatics	0,983614	0,000162	-8,4E-07	-0,00043	-1,9E-06	-0,00062	8,02E-06	-0,0004	3,89E-06	-0,00245	1,54E-06	-0,01873	0,010051
C42 Aromatics	0,493958	3,66E-05	-3,9E-06	-3,4E-05	-2,4E-06	-0,00015	2,51E-06	-0,00015	3,55E-06	-0,0012	7,39E-07	-0,00529	0,003173
CO	0,086284	-9,7E-06	-1,1E-06	-5,5E-05	-2,7E-07	-7,2E-05	1,71E-07	-6,9E-05	4,94E-07	-0,00024	1,7E-07	0,00616	-0,00223
CO2	0,056984	-3,9E-06	-8,2E-07	-2,3E-05	-7,2E-07	-3,9E-05	2,26E-07	-3,5E-05	1,8E-07	-0,00015	9,59E-08	0,0019	-0,00041

Table 6-7: coefficients of polynomial reactor model 5

Component	Intercept	C2	C2²	COT	COT²	STR²	STR²
H2	-0,82661	-0,00188	5,28E-05	0,001857	-9,6E-07	0,000169	-0,0021
CH4	2,026693	-0,00897	0,000402	-0,00551	3,85E-06	-0,03779	0,016214
C2H2	0,447936	-5,6E-05	-3E-06	-0,00118	7,76E-07	0,00298	-0,00072
C2H4	-16,5184	-0,01224	0,000141	0,03906	-2,2E-05	0,015594	-0,03372
C2H6	14,10293	0,033554	-0,00104	-0,02929	1,5E-05	0,049149	0,00956
C3H6	-0,57875	-0,00113	4,36E-05	0,001365	-7,8E-07	-0,00745	0,002673
C3H8	-0,10035	-6,2E-05	2,36E-06	0,000239	-1,4E-07	-0,00071	0,000305
NBUTA	-0,28248	0,000105	-3,8E-06	0,000722	-4,6E-07	-0,00139	0,000448
B1	-0,05251	-2,9E-05	7,71E-07	0,000126	-7,4E-08	-0,00042	0,000156
BUTAD	0,057919	-0,00055	7,49E-06	-0,00029	2,86E-07	0,001342	-0,00184
BENZ	1,168247	-0,0037	0,000165	-0,00305	2,03E-06	-0,01067	0,004079
TOLUO	0,102284	-0,00032	1,34E-05	-0,00027	1,84E-07	-0,001	0,000341
STYR	0,381388	-0,00091	4,3E-05	-0,00097	6,29E-07	-0,00262	0,001173
FUEL1	0,181534	-0,0005	2,29E-05	-0,00047	3,07E-07	-0,00139	0,000531
CPTD	-0,15577	-0,00028	1E-05	0,000368	-2,1E-07	-0,00119	0,000226
CC5H8	-0,10308	-0,00011	3,08E-06	0,00025	-1,5E-07	-0,00086	0,000228
C4H4	0,097301	-4,7E-05	1,07E-06	-0,00025	1,63E-07	0,000308	-0,00014
FUEL3	0,242729	-0,00056	2,65E-05	-0,00062	4,01E-07	-0,00163	0,000703
FUEL4	0,043046	-9,3E-05	4,44E-06	-0,00011	7,01E-08	-0,00026	0,000118
FUE43	0,040304	-9,6E-05	4,79E-06	-0,0001	6,47E-08	-0,00027	0,000142
PES32	0,4053	-0,00096	4,73E-05	-0,00103	6,56E-07	-0,00276	0,001381
PES42	0,196844	-0,00051	2,61E-05	-0,00049	3,14E-07	-0,00148	0,000841
CO	0,11544	-0,00022	8,87E-06	-0,00031	2,08E-07	0,003196	-0,00118
CO2	0,032059	-0,00013	6,1E-06	-8,4E-05	5,59E-08	0,000764	-7,4E-06

Table 6-8: coefficients of polynomial reactor model 6

Component	Intercept	Naphtha 1	Naphtha 1²	COT	COT²	STR²	STR²
Hydrogen	-0,07448	-9,8E-05	7,43E-07	0,000164	-7,4E-08	0,000535	-0,00079
Methane	-1,26169	-0,00267	2,8E-05	0,002906	-1,4E-06	-0,07843	0,030275
Acetylene	0,195272	-1,8E-05	-1,5E-07	-0,00053	3,59E-07	0,003476	-0,00158
Ethylene	-3,22546	-0,00193	1,04E-05	0,007461	-3,9E-06	0,030937	-0,0406
Ethane	-0,48385	-0,00038	5,57E-06	0,001308	-7,9E-07	-0,05066	0,028592
Propadiene	0,080919	3,92E-06	-7E-07	-0,00026	2,1E-07	0,004767	-0,00264
Propylene	-4,8886	0,001081	-1,9E-05	0,012471	-7,7E-06	0,024607	-0,02808
Propane	-0,09427	2,13E-05	3,34E-07	0,000264	-1,7E-07	-0,0075	0,004324
n-Butane	0,073495	9,92E-05	-8,9E-07	-0,00014	6,61E-08	0,002049	-0,0005
i-C4=	-1,16899	0,000611	-7,9E-06	0,003109	-2E-06	0,010406	-0,00866
1-C4=	-0,54362	0,000629	-7,3E-06	0,001492	-1E-06	0,01531	-0,00659
2-C4=	-0,24408	0,000298	-3,5E-06	0,000711	-5E-07	0,005609	-0,00376
1,3-C4==	-1,75501	0,000817	-1,3E-05	0,004304	-2,6E-06	0,039721	-0,02781
Benzene	-0,29754	-0,00226	2,49E-05	0,000465	5,81E-08	-0,06711	0,029569
Toluene	-0,45428	-0,00093	1,02E-05	0,001063	-5,4E-07	-0,0333	0,015828
Xylene	-0,08397	5,39E-05	-4,6E-07	0,00028	-2E-07	-0,00167	0,001317
Ethylbenzene	-0,02897	3,11E-05	-3,2E-07	8,72E-05	-6,1E-08	0,000349	-1,3E-05
Styrene	0,215181	-0,00036	4,26E-06	-0,00057	3,98E-07	-0,00935	0,004645
C9 Aromatics	0,238151	0,00023	-1,9E-06	-0,00049	2,39E-07	0,003892	-0,00057
n-C5	0,834579	0,000523	-4,4E-06	-0,00187	1,03E-06	0,01392	-0,00291
i-C5	0,685921	0,000436	-3,7E-06	-0,00153	8,35E-07	0,011169	-0,00233
n-C8	0,758962	0,000198	-1,1E-06	-0,00179	1,05E-06	0,005517	0,000306
n-C9	0,467197	0,000101	-4,2E-07	-0,00111	6,53E-07	0,002824	0,000492
n-C10	0,129146	2,35E-05	-6,3E-08	-0,00031	1,82E-07	0,00066	0,00021
Cyclo-C5	0,159136	8,71E-05	-7,2E-07	-0,00036	2,05E-07	0,002475	-0,00045
Methylcyclo-C5	0,362351	0,000152	-1,1E-06	-0,00084	4,83E-07	0,004346	-0,00046
Cyclo-C6	0,621106	0,000277	-2,1E-06	-0,00144	8,24E-07	0,008081	-0,00102
C7 Naphthene	2,415732	0,000705	-4,1E-06	-0,00568	3,31E-06	0,019766	0,000569
C8 Naphthene	0,568006	0,000121	-4,8E-07	-0,00135	7,94E-07	0,003372	0,00064
2-M-C4=	0,122956	7,29E-05	-6,5E-07	-0,00027	1,5E-07	0,001598	-0,00054
1-C5=	0,263065	9,94E-05	-7,6E-07	-0,00061	3,46E-07	0,001816	-0,00034
Naphthalene	0,199996	-0,00057	6,56E-06	-0,00057	4,35E-07	-0,0171	0,008561
1-M-C4=	-0,01514	0,000201	-2E-06	9,68E-05	-9,8E-08	0,004777	-0,00153
Dimethylcyclo-C6	0,036323	1,12E-05	-1,2E-07	-7,9E-05	4,31E-08	-0,00028	0,000131
i-C10	0,16837	2,87E-05	-5,8E-08	-0,0004	2,38E-07	0,000798	0,000294
C5==	-0,03468	0,000176	-2,1E-06	0,000125	-9,9E-08	0,004961	-0,00279
Isoprene	-0,38372	0,000314	-3,9E-06	0,001018	-6,7E-07	0,007621	-0,00459
i-C6=	0,036438	5,01E-05	-4,9E-07	-7,1E-05	3,22E-08	0,001107	-0,00034
Methylcyclo-C6	0,0975	2,95E-05	-2,4E-07	-0,00022	1,19E-07	-0,00019	0,0003
i-C6	2,515484	0,000923	-6,4E-06	-0,00583	3,35E-06	0,024337	-0,00222
1,3-C6==	0,090854	3,11E-05	-2,6E-07	-0,00021	1,2E-07	0,000528	-0,00015
1,3-M-C5==	-0,15586	0,000101	-1,3E-06	0,000412	-2,7E-07	0,002192	-0,00149
C7 Aromatics	0,231207	7,03E-05	-5E-07	-0,00054	3,15E-07	0,001802	-0,00024
M-Cylco-C5=	0,173539	5,36E-05	-4,3E-07	-0,0004	2,26E-07	0,000338	-2,2E-05
i-C7	2,316465	0,000659	-3,9E-06	-0,00544	3,16E-06	0,017733	1,25E-05
M-C6==	0,017345	6,18E-05	-6,6E-07	-1,4E-05	-8E-09	0,000994	-0,00052
Cylco-C5==	-1,23997	0,000149	-2,9E-06	0,0031	-1,9E-06	0,002557	-0,00452

C8 Aromatics	0,120304	3,14E-05	-2E-07	-0,00028	1,66E-07	0,000841	-4,3E-05
Cylco-C5=	-0,159	3,66E-05	-5,7E-07	0,000427	-2,8E-07	-0,00115	-1,9E-05
i-C8	1,209284	0,000284	-1,4E-06	-0,00286	1,68E-06	0,00777	0,000787
i-C9	0,456771	9,06E-05	-3,2E-07	-0,00109	6,41E-07	0,002509	0,000556
Cyclo-C6=	0,249686	6,22E-05	-4,1E-07	-0,00058	3,35E-07	0,00098	-3,7E-05
C4H4	0,036282	-1E-05	7E-08	-9,6E-05	6,44E-08	0,000372	-0,00027
M-Styrene	-0,09144	-0,00011	1,27E-06	0,000227	-1,3E-07	-0,00513	0,002578
Dimethylstyrene	0,00408	-6,7E-06	1,08E-07	-5,8E-06	2,95E-09	-0,00054	0,000367
C16H12 Aromatics	0,21693	-0,00049	5,83E-06	-0,00059	4,33E-07	-0,01442	0,007728
M-Cylco-C5==	-0,34052	0,000122	-1,7E-06	0,000893	-5,8E-07	0,001387	-0,00153
M-Cyclo-C6==	0,024542	1,36E-05	-1,9E-07	-4,6E-05	2,06E-08	-0,00053	0,000129
Indene	-0,05009	-0,00014	1,66E-06	0,000113	-5,1E-08	-0,00556	0,002916
C22 Aromatics	0,041971	-8E-05	9,76E-07	-0,00011	7,7E-08	-0,00257	0,001419
C7==	0,005125	1,89E-05	-2,2E-07	-9,1E-07	-6,2E-09	-2,2E-05	-9,8E-05
C40 Aromatics	0,007545	-4E-05	4,88E-07	-2,2E-05	1,93E-08	-0,0015	0,000845
C32H20 Aromatics	0,383358	-0,00046	5,86E-06	-0,00099	6,66E-07	-0,01364	0,00812
C42 Aromatics	0,084568	-7,7E-05	1E-06	-0,00022	1,41E-07	-0,00206	0,001266
2-C5=	0,139242	0,000142	-1,4E-06	-0,00029	1,43E-07	0,003104	-0,00115
1-C6=	0,202974	5,58E-05	-3,6E-07	-0,00048	2,79E-07	0,001312	-0,00017
2-M-C5=	0,15298	5,81E-05	-4,5E-07	-0,00035	2,03E-07	0,001388	-0,00033
1-C8=	0,062841	1,7E-05	-1,1E-07	-0,00015	8,67E-08	0,000456	-4,3E-05
1-M-C4=	0,067033	0,000107	-1E-06	-0,00013	5,25E-08	0,002138	-0,00083
C6==	0,100973	2,3E-05	-1,4E-07	-0,00024	1,4E-07	0,000527	-7,9E-05
1-M-C5=	0,18442	3,49E-05	-2E-07	-0,00044	2,59E-07	0,000751	-6,5E-05
1-C7=	0,140747	3,32E-05	-2E-07	-0,00033	1,96E-07	0,000825	-0,00011
CO	0,042653	-4,1E-05	4,33E-07	-0,00012	8,4E-08	0,002501	-0,00109

6.2 Reactor model comparison

6.2.1.1 abs. deviation to simulation – validation case 1
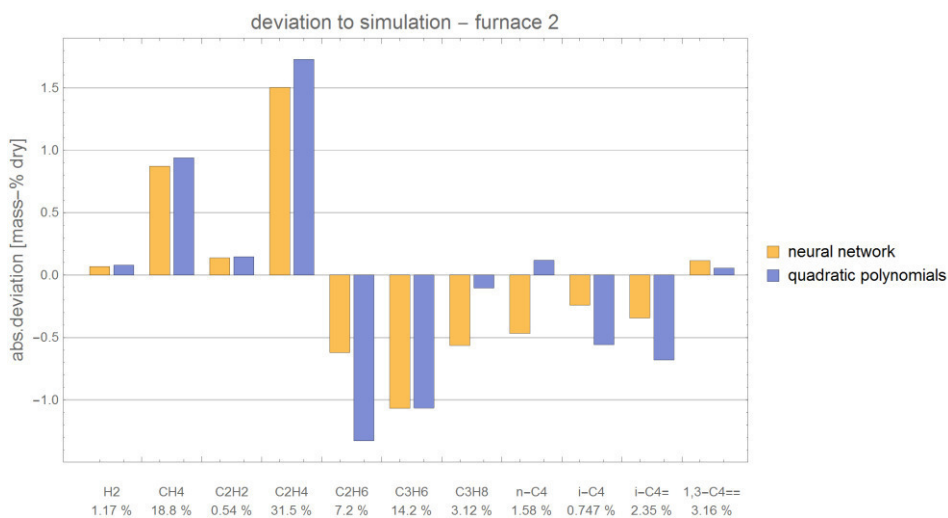
Figure 6-1: abs. deviation to simulation - furnace 2 (case 1)
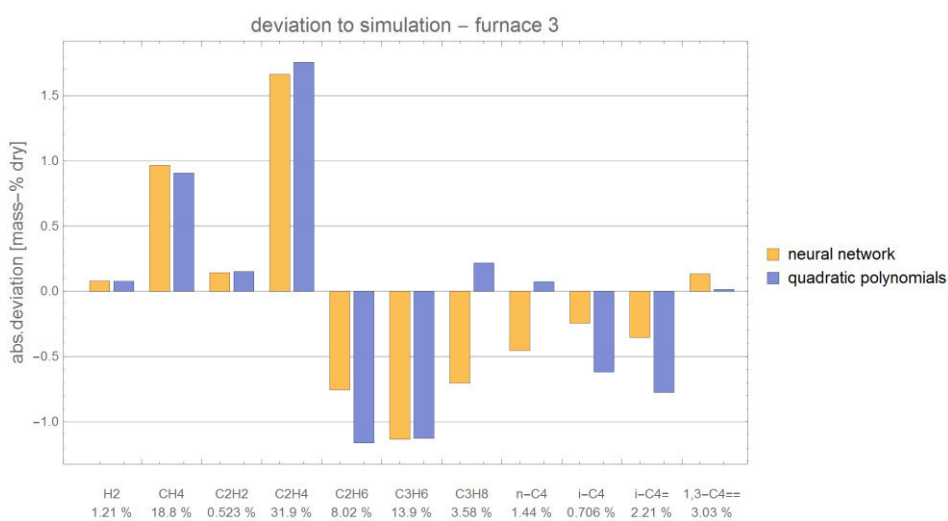
Figure 6-2: abs. deviation to simulation - furnace 3 (case 1)
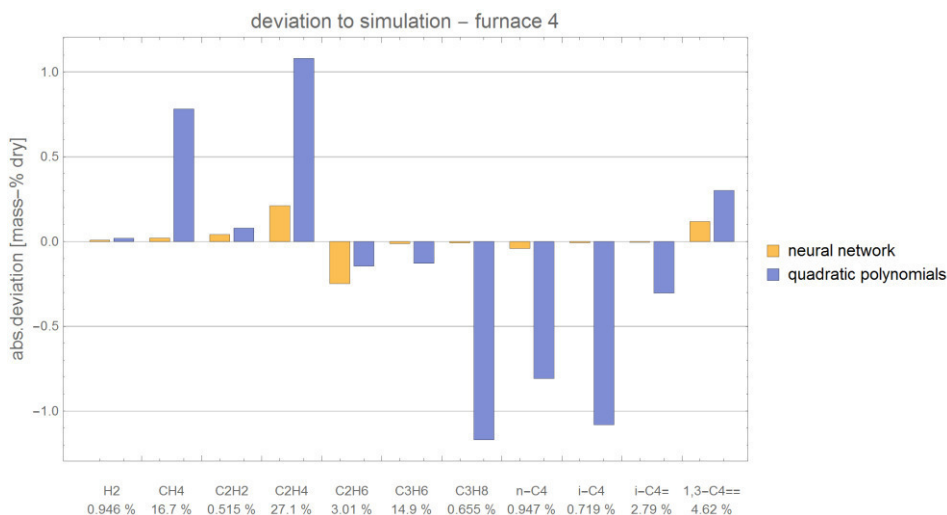
Figure 6-3: abs. deviation to simulation - furnace 4 (case 1)
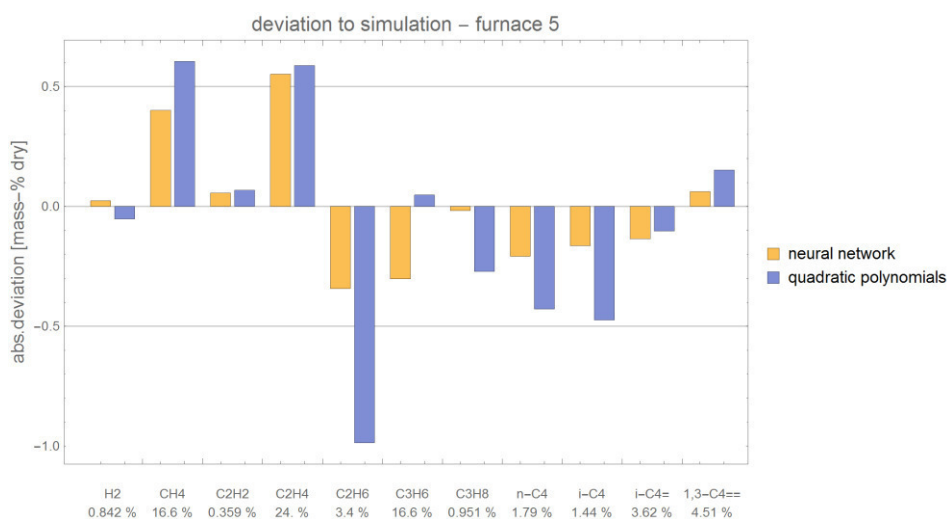
Figure 6-4: abs. deviation to simulation - furnace 5 (case 1)
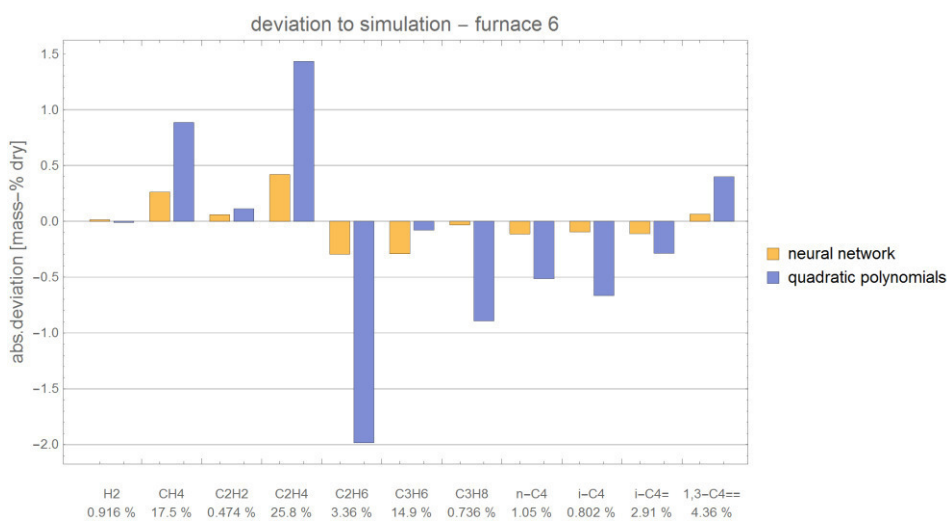
Figure 6-5: abs. deviation to simulation - furnace 6 (case 1)
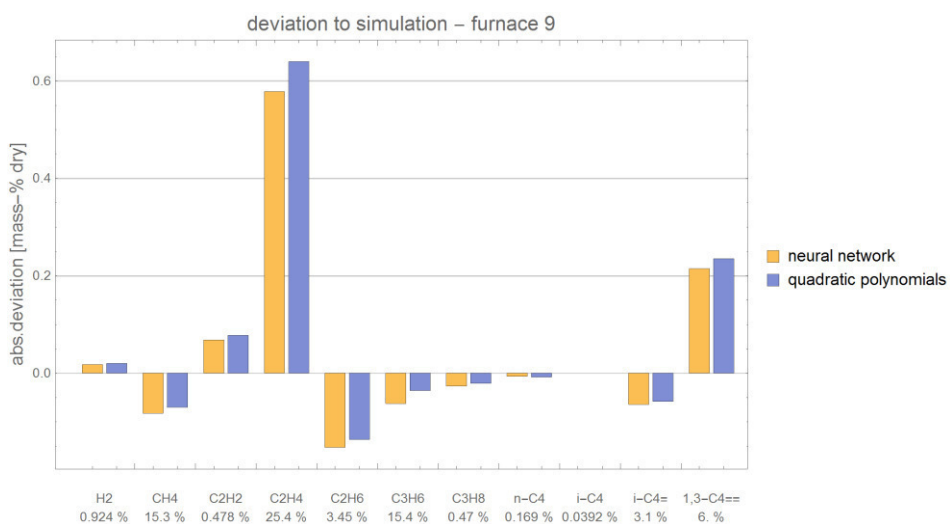
Figure 6-6: abs. deviation to simulation - furnace 9 (case 1)
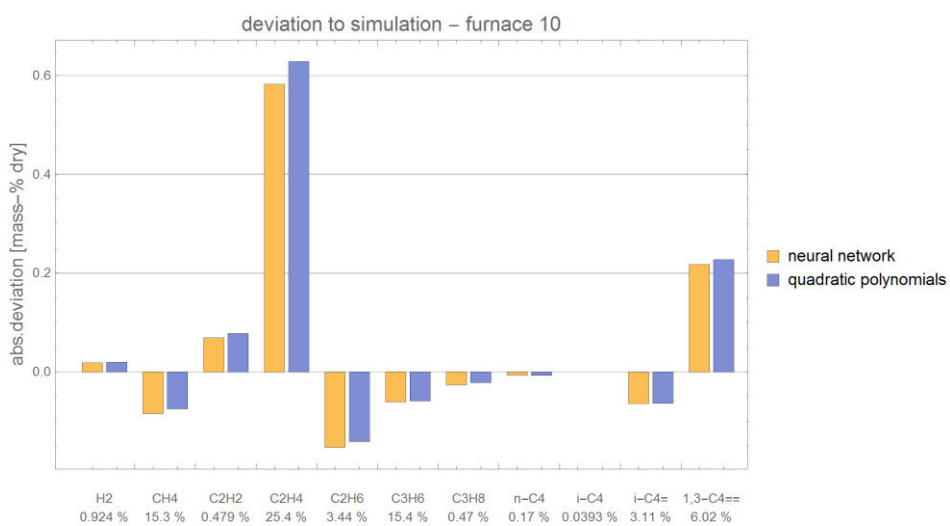
Figure 6-7: abs. deviation to simulation - furnace 10 (case 1)

6.2.1.2   abs. deviation to simulation – validation case 2
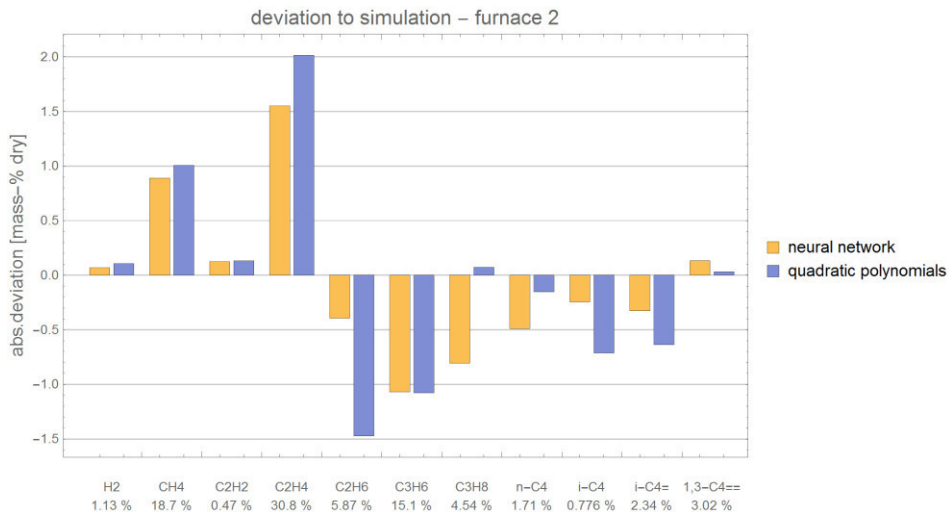
Figure 6-8: abs. deviation to simulation - furnace 2 (case 2)
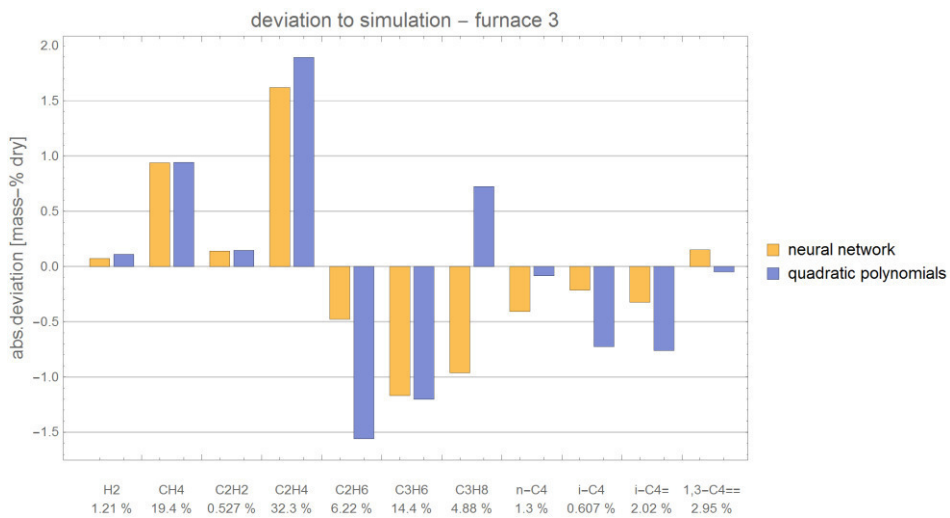
Figure 6-9: abs. deviation to simulation - furnace 3 (case 2)
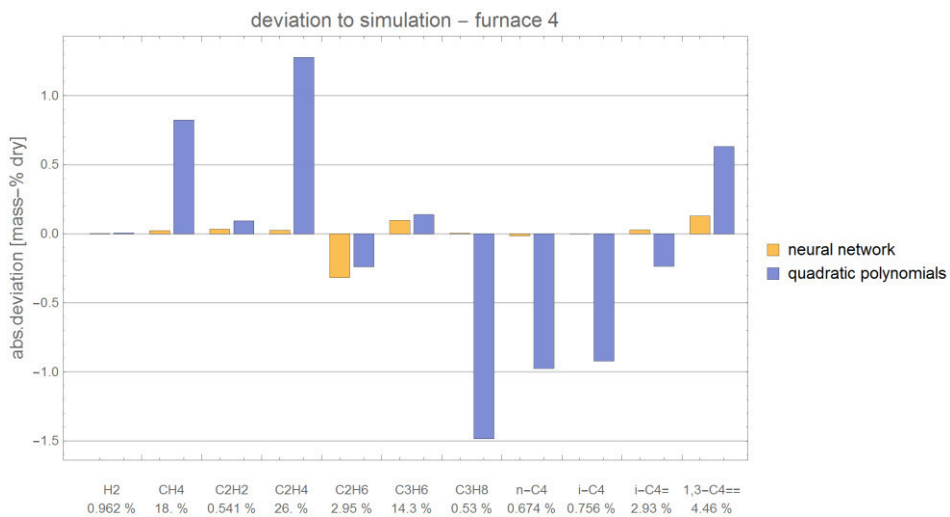
Figure 6-10: abs. deviation to simulation - furnace 4 (case 2)
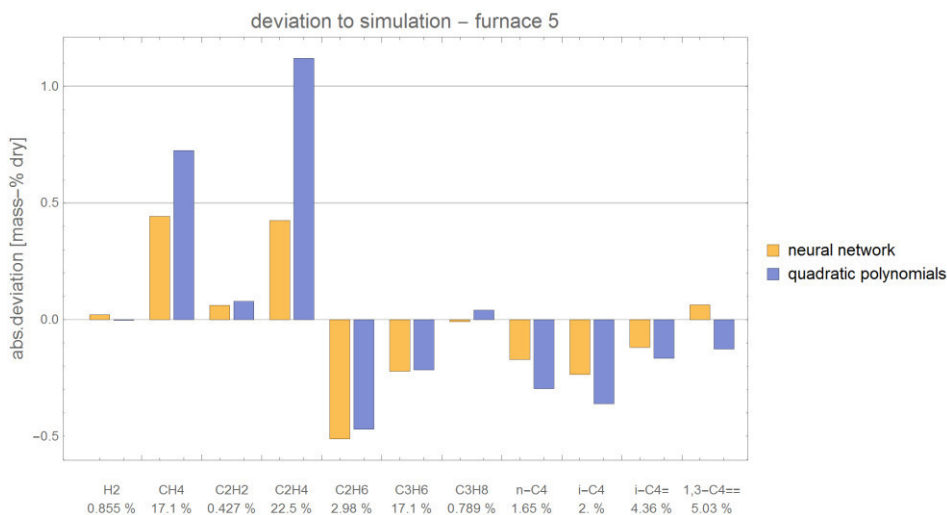
Figure 6-11: abs. deviation to simulation - furnace 5 (case 2)
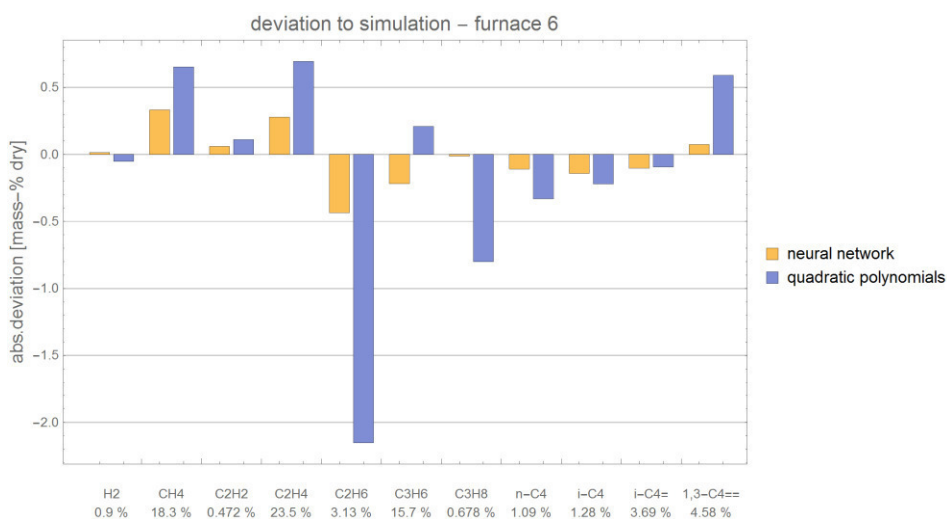
Figure 6-12: abs. deviation to simulation - furnace 6 (case 2)
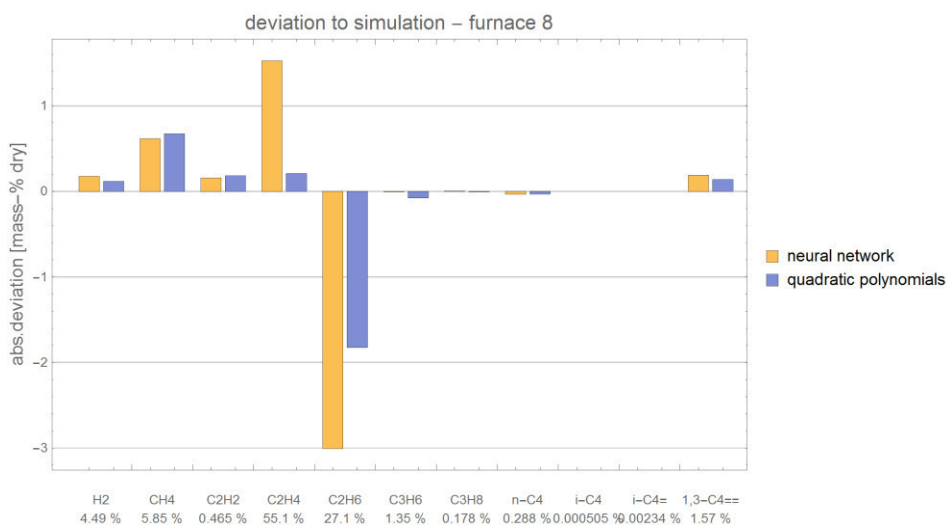
Figure 6-13: abs. deviation to simulation - furnace 8 (case 2)
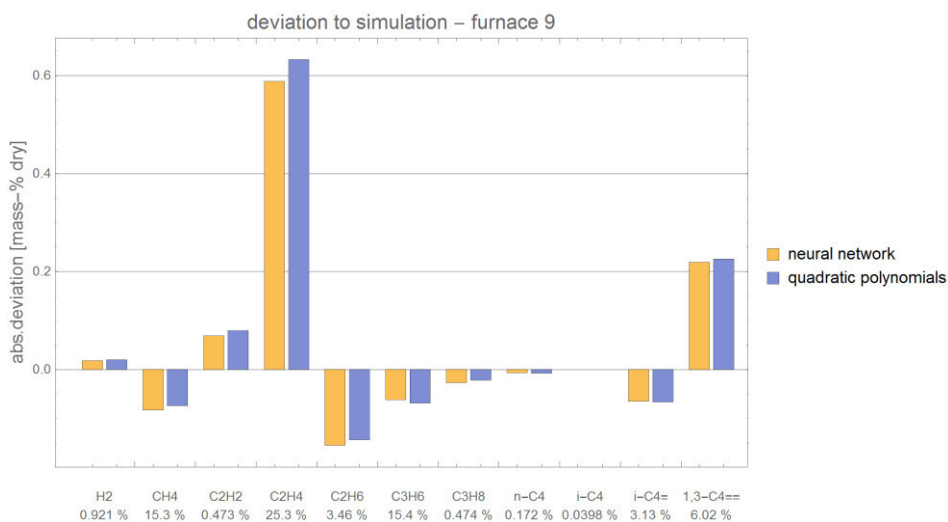
Figure 6-14: abs. deviation to simulation - furnace 9 (case 2)
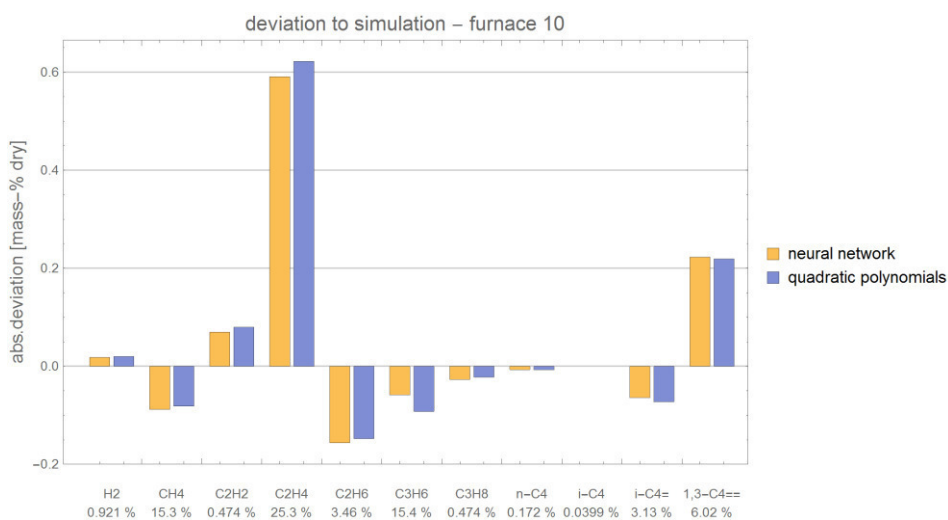
Figure 6-15: abs. deviation to simulation - furnace 10 (case 2)

6.2.1.3   abs. deviation to simulation – validation case 3
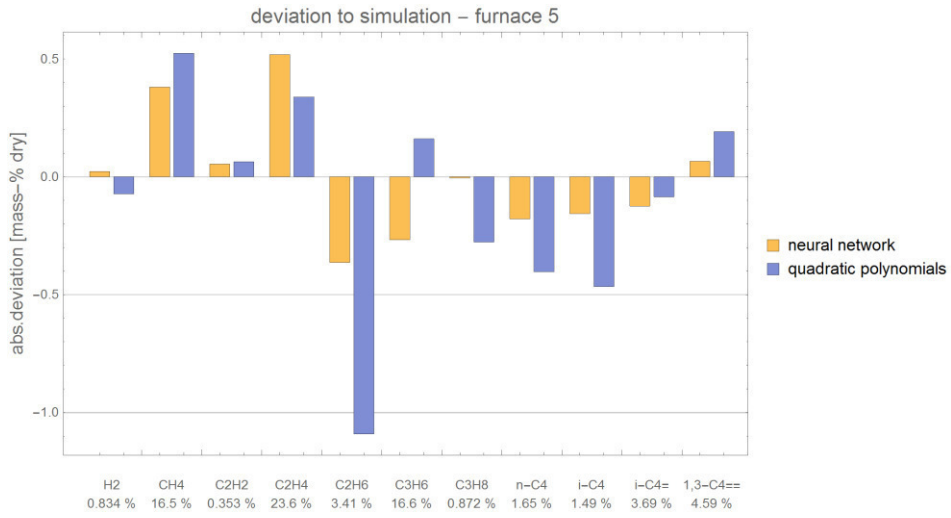
Figure 6-16: abs. deviation to simulation - furnace 5 (case 3)
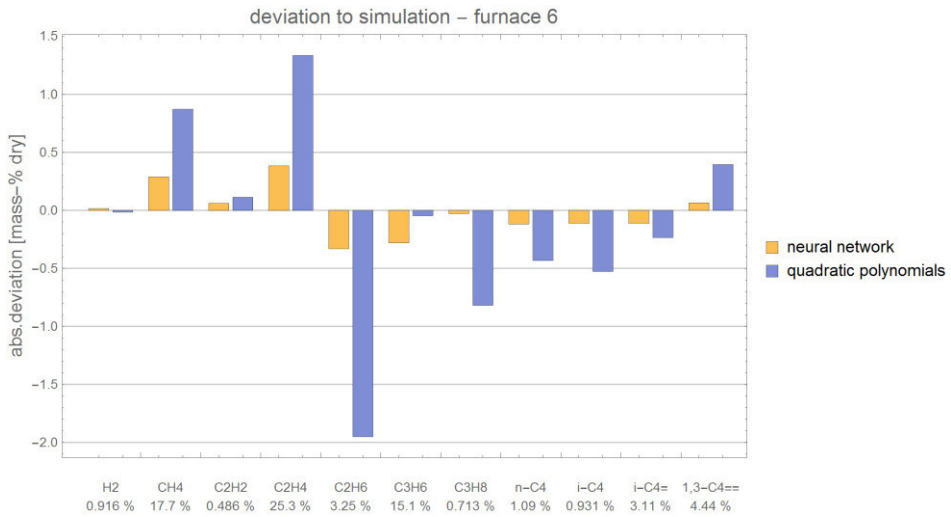
Figure 6-17: abs. deviation to simulation - furnace 6 (case 3)
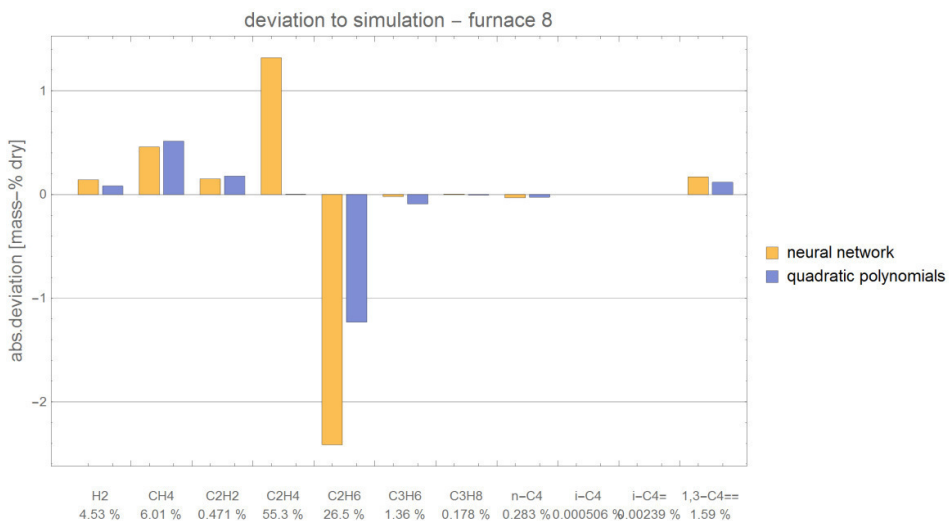
Figure 6-18: abs. deviation to simulation – furnace 8 (case 3)
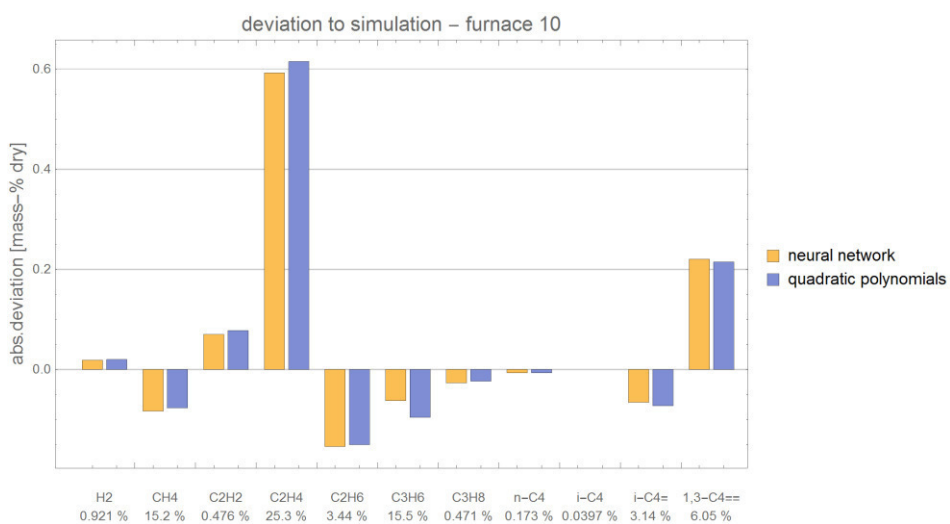
Figure 6-19: abs. deviation to simulation - furnace 10 (case 3)

6.3 Symbols

Symbol	Unit	Description
p	bar	Pressure
T	°C	Temperature
x	kg/kg	Mass fraction
X		Predictor variables
Y		Response variables
COT	°C	Coil outlet temperature
STR	kg/kg	Steam dilution ratio
MF	t/h	Mass flow of hydrocarbons

Abbreviations	Description
n-C4	n-Butane
i-C4	i-Butane
iC4=	i-Butene
1,3-C4==	1,3-Butadiene

Dubscripts

i,j,k	Counter variables

6.4   Figures

6.5 Tables

6.6 Literature

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