DEVELOPMENT OF A MODEL PREDICTIVE CONTROLLER OF HYDROTREATING REACTOR CO-FEEDING BIOBASED FEED

Lappeenranta–Lahti University of Technology LUT

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ABSTRACT

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Development of a Model Predictive Controller of hydrotreating reactor co-feeding biobased feed

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Biofuels are one important solution to reduce traffic CO_2 emissions and gradually reduce our dependence on fossil oil. Stand-alone biofuel production facilities are expensive investments, and one interesting option to reduce costs is to use current petroleum refinery infrastructure to co-process biomass-derived feedstock with petroleum fractions in the refinery process units. The product of co-processing is hybrid fuel with bio-content,

Hydroprocessing units operate in high hydrogen partial pressure and temperatures. The reactors and catalytic reactions in those are suitable for oxygen removal reactions and hydrogenation of triglycerides to be suitable for diesel fuel production.

A significant difference comparing bio-based and petroleum feedstocks is the high oxygen content in bio-feed. Oxygen removal reactions in a hydrotreating reactor cause increased exothermic reactions, and CO, CO_2 and H_2O byproducts.

One efficient tool to optimise efficient production in process units is the Model Predictive Controller (MPC). It can operate selected controlled variables close to process constraints, which is often the optimal operating method.

The thesis work subject was to design and implement an MPC controller for a petroleum refinery hydrotreating unit reactor. The future plan is to start co-processing in this process unit, and advanced reactor temperature control will improve the operationality of the reactor in constrained situations, like increased reactor exotherms.

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Lappeenrannan–Lahden teknillinen yliopisto LUT

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Kemiantekniikka

Jukka Viertorinne

Mallipredikatiivisen monimuuttujasäätimen kehitys vetykäsittelyreaktoriin, jonka syöttönä raakaöljyn tislausjae ja bioperäinen syöttö-öljy

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Biopolttoaineet ovat tärkeä tekijä liikenteen CO_2 päästöjen vähentämiseksi. Niiden tuotantoa lisäämällä ja tuotantomenetelmiä kehittämällä voidaan asteittain pienentää riippuvuuttamme fossiiliperäisestä raakaöljystä. Biopolttoaineiden tuotantolaitokset ovat suuria ja kalliita investointeja. Mahdollinen keino kustannusten laskemiseksi on nykyisten raakaöljyjalostamoiden tuotantoyksiköiden käyttäminen myös biopolttoaineiden valmistamiseen. Yksi keino tähän on bioperäisen ja raakaöljypohjaisen syötön yhteiskäsittely, jolloin tuote on hybridi polttoaine biokomponentilla.

Vetykäsittely-yksiköt toimivat korkessa vedyn osapaineessa ja lämpötilassa. Näiden tuotantoyksiköiden reaktorit ja niissä tapahtuvat vedytysreaktiot soveltuvat mm. hapenpoistoon sekä triglysereiden vedyttämiseen dieseljakeeseen soveltuviksi hiilivedyiksi.

Merkittävä ero vertaillessa biosyöttöaineita ja fossiilista öljyä on bioperäisten syöttöaineiden korkea happipitoisuus. Lisääntyneet hapenpoistoreaktiot nostavat reaktorin lämmönnousua eksotermisten reaktioiden määrän lisääntyessä. Sivutuotteina hapenpoistosta tulee häkää, hiilidioksidia ja vettä.

Tehokas työkalu prosessiyksikön tuotannon optimointiin on mallipredikatiivinen säädin (MPC), jonka avulla prosessiyksikköä voidaan operoida tehokkaasti prosessirajoitteita vasten, jolloin tuotanto on yleensä tuottoisinta. Lopputyön aiheena oli suunnitella ja käyttöönottaa MPC säädin vetykäsittelyreaktoriin, jonka syöttöaineeksi on tulevaisuudessa tulossa bioperäistä syöttöainetta fossiilisen syötön lisäksi. Kehittyneemmällä reaktorin lämpötilan säädöllä voidaan reaktoria hallita paremmin rajoittuneissa operointitilanteissa, esimerkiksi eksotermisten reaktioiden lisääntyessä.

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ABBREVIATIONS

APC	Advanced Process Controller
CAPEX	Capital Expenditure
CCR	Conradson Carbon Residue
CFPP	Cold Filter Plugging Point
CHAZOP	Hazards and Operability
CoMo	Cobalt Molybdenum
CV	Controlled Variable
DCS	Distributed Control System
DCS	Distributed Control System
FAME	Fatty Acid Methyl Ester
FCC	Fluid Catalytic Cracking
FF	Feed-Forward Variable
FIR	Finite Impulse Response
FMEA	Failure Mode Analysis
FSR	Finite Step Response
GHG	Green House Gas
HDC	Hydrocracking
HDM	Hydrometallization
HDN	Hydrodenitrogenation
HDN	Hydrodenitrogenation
HDO	Hydrodeoxygenation
HDS	Hydrodesulfurization

HDT	Hydrotreating
HVO	Hydrotreated Vegetable Oil
HYD	Hydrogenation
IDCOM	Identification Command
LSS	Linear State-Space
MAC	Model Algorithmic Control
MEROX	Mercaptan Oxidation
MIMO	Multiple Input Multiple Output
MOC	Management of Change
MTBE	Methyl tert-Butyl Ether
MV	Manipulated Variable
NiMo	Nickel Molybdenum
OPEX	Operating Expence
PAS	Process Automation System
PID	Proportional-Integral-Derivative Controller
PV	Process Value
RED	European Renewable Energy Directive
RTO	Real Time Optimization
SP	Setpoint
TBR	Trickle-Bed Reactor
UCO	Used Cooking Oil
VGO	Vacuum Gas Oil
WABT	Weighted Average Bed Temperature

Table of contents

Contents

1 Introduction

Climate warming caused mainly by increasing CO_2 and other greenhouse gases (GHG) levels in atmosphere and other fossil fuels related problems has awakened politicians, scientists, and industry to seek alternatives for the fossil crude oil and its products. The European Commission 2030 Climate Target Plan aims to reduce GHG emissions to at least 55% below 1990 levels (European Commission).

One means to achieve the target are biofuels, that can replace, e.g., traffic fossil fuels like naphtha and diesel, and are suitable to be used in current combustion engines without modifications. Traditional oil refineries can be potential production facilities for biofuels and low-carbon fuels using existing process equipment.

The subject of this thesis is the development of an advanced process controller (APC-controller) to improve the temperature controllability of a hydrotreating reactor, which is planned to start co-processing biobased feed. The controller should be able to control and keep the reactor at selected temperature targets, manipulating Distributed Control System (DCS) temperature controllers. There are also constraints that affect temperature control, which the controller needs to handle. Controller strategy and structure need inputs also from users, panel operators and plant engineers. The controller design phase, related tests, and implementation are done in close cooperation with users.

1.1 Background of the work

Global warming is increasing mainly because of human activities that generate gases like carbon dioxide, methane, and nitrous oxides (Kazancoglu, Ozbiltekin-Pala and Ozkan-Ozen, 2021). Advanced biofuels are one of the options and possibilities to reduce transport sector emissions. As Panoutsou et al. (2021) point out, this is especially important for aviation, marine and heavy-duty vehicles, which do not currently have efficient alternatives.

New stand-alone biofuel production sites are significant investments, and economic challenges related to higher fuel pricing compared to fossil fuels and changing mixing mandates and policies can reduce the interest towards investments. Current petroleum refineries are one option to reduce needed investment costs, as the refineries often have extensive processing infrastructure and utilities required. Processing a mixture of biobased and fossil feed in the same processing unit can produce ready fuel or fuel components with bio-share.

Some of the possible processing limitations can be handled with Advanced Process Controllers (APC), pushing the process against process limitations to increase the benefits and maximise production.

1.2 Goals and benefits

The goal of the work is enhanced reactor temperature control, including controller design, step testing and modelling, operator training and implementation. Currently the unit panel operator controls the reactor temperature with DCS-control loops. This requires constant operator follow-up as the temperatures, reactor exotherms, and hydrogen flows change. Advanced reactor control should reduce temperature fluctuations and ease operator work. The main benefits come from reduced temperature fluctuations and more precise and better control in constrained situations, e.g. high reactor bed temperature rice or cooling gas valve opening limits. With an advanced process controller, the process can be operated closer to process limitations gaining more production benefits that can be e.g. feed increase, improved energy efficiency or smaller fluctuations in product quality (King, 2011).

1.3 Structure and delimitations

The thesis work included the design of controller structure, functional design, process testing, development of process models, controller-related configuration work, operator training and controller implementation. The scope did not include the distributed control system (DCS) and process history system related configuration work.

2 Biomass

Biomass is a generic term for all materials that are derived from growing plants (Sillanpää and Ncibi, 2017). As it is constantly renewing, there are enormous sources of biomass, and it can replace fossil fuels. This chapter handles the biomass that can be used in biofuel production and the many forms the biomass appears.

2.1 Biomass in general

The basic biologically definition for biomass is that it originates from growing plants. The industry and engineers in bioeconomy sector are widening the definition also to biomass sources like algae, agro-industrial by products and food wastes and municipal wastes (Sillanpää and Ncibi, 2017). It appears in different forms like oil, fats, starch, and lignocellulose (Morales, Iglesias and Melero, 2020) wide range of end products and energy. The European Commission (Directive 2009/28/EC) has the following definition for biomass: "*the biodegradable fraction of products, waste and residues from biological origin from agriculture (including vegetal and animal substances), forestry and related industries including fisheries and aquaculture, as well as the biodegradable fraction of industrial and municipal waste*".

Important factor related to biomass and the usage of it e.g., in biofuel production is the sustainability. The used biomass should not be material, that could be used in food production (Morales et. al. 2020) or cause negative effects via land-use change.

2.2 Biomass classification

As the term biomass encompasses large variety of plants and fractions of plants, different transformation residues and wastes, there has been multiple attempts to group and categorize different biomass recourses. Dividing into different categories has been made by number of different factors, like based by the origin (land/water), production (forest/agricultural/waste), biochemical composition or end-use purpose (energy/chemicals/materials).

Sillanpää and Ncibi (2017) has grouped the biomass in woody, herbaceous, aquatic, and wastes and residues and classified in three classes (Figure 1) depending on the biomass source:

- Natural resources, biomass is harvested
- Cultivation, and harvesting
- Transformation, biomass from residues and wastes

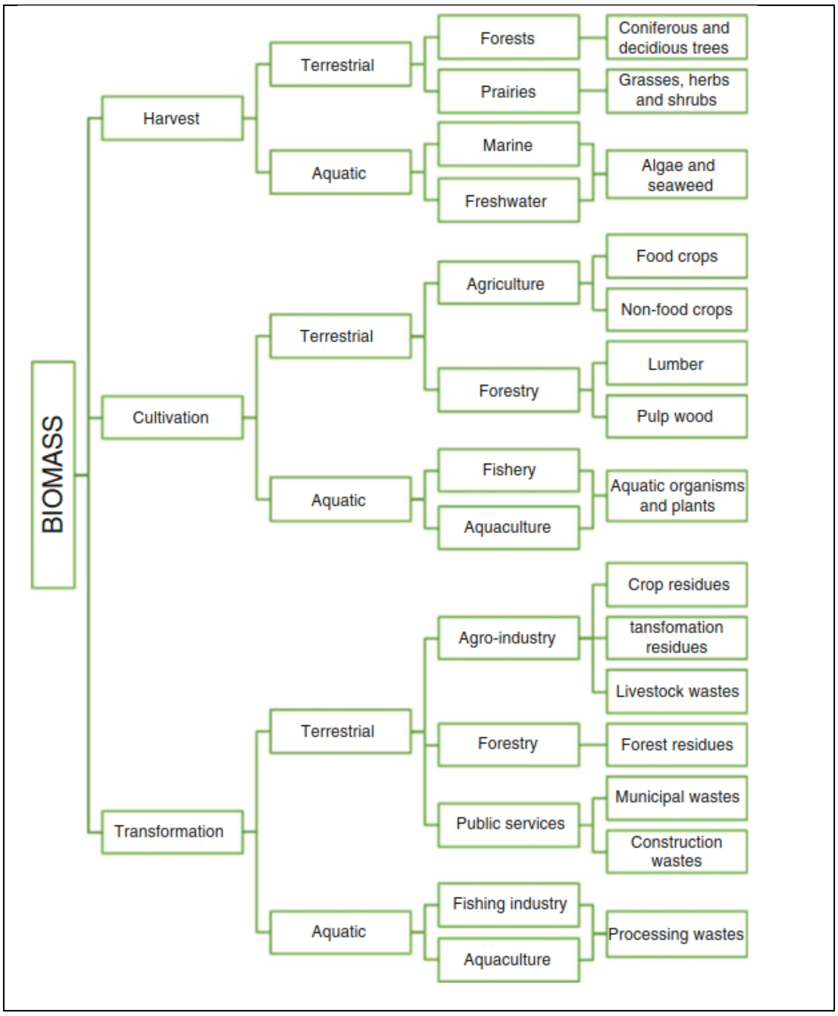


Figure 1 Biomass classification (Sillanpää and Ncibi, 2017)

Natural biomass sources grow naturally, compared to cultivation, where the biomass is cultivated first, and harvested later. The use of different wastes as raw material source is important. E.g. agricultural sector leaves large fraction of biomass unused, like cereal plant straws and corn stowers (Sillanpää and Ncibi, 2017).

2.2.1 Woody biomass

Woody biomass includes bark, wood, roots, leaves, stumps, and needles. It can be derived from manufacturing and processing factories and used waste wood (Alakangas, Valtanen and Levlin, 2006). Forest management, like thinning young stands, removing dead trees and cutting older trees for pulp and lumber, produces woody biomass for the biomass market. Also, the plantation of fast-growing trees for the energy sector provides woody biomass (Sillanpää and Ncibi, 2017).

As the main composition of wood is cellulose, hemicellulose and lignin, the terms woody and lignocellulosic biomass are sometimes used as synonyms, which is not accurate, as the lignocellulosic biomass is wider ranging as it also includes other plants composed of lignin and cellulose, like herbaceous biomass (Sillanpää and Ncibi, 2017)

Lignocellulosic biomass is an inexpensive feed source, and the efficient valorisation of this abundant feed source material would open the possibilities to produce bio-products in an inexpensive, eco-friendly, and renewable way. The main components of lignocellulosic biomass are cellulose, hemicellulose, and lignin (Sillanpää and Ncibi, 2017). The proportion of the main component varies based on the biomass and the part of the plant. Wood generally contains 40-45% cellulose, hemicellulose 20-30%, and lignin 26-32% (Sjöström, 1993).

The main problem, which has not been fully solved yet, is the protected structure of lignocellulosic material and how to break it in an economically and sustainable way. Lignin forms a protective covering, that makes cellulose and hemicellulose recalcitrant against e.g. enzymatic hydrolysis (Bajpai, 2016). Enzymatic hydrolysis is a process that can be used to convert cellulosic biomass into fermentable sugars that can be used e.g. to produce bioethanol. Recalcitrant components in lignocellulosic biomass require expensive pre-treatment steps before main processing and further optimisation is still needed to increase yields at lower cost (Sillanpää and Ncibi, 2017).

2.2.2 Herbaceous biomass

Herbaceous plants are an exciting biomass source as they have the most extensive annual biomass stock and are fast renewable. Herbaceous plants are grouped as:

- Natural herbaceous plants like grasses and forbs.
- Agricultural crops like wheat, corn, rice and flax and energy crops like Reed Canary Grass.
- Agro-industrial residues are the fractions of the crop left on the field after harvesting. Cereal straws and corn stover are examples of this group (Sillanpää and Ncibi, 2017).

2.2.3 Aquatic biomass

Seagrasses, micro and macro algae, and other plants growing or planted in aquatic environments are classified as aquatic biomass. Aquatic biomass can grow in lakes, seas, ponds and rivers (Sillanpää and Ncibi, 2017) . It does not compete with food production and does not require large land areas for cultivation.

Algae is an interesting aquatic biomass source, e.g. for biodiesel production. It can be cultivated in open ponds or closed tanks, bioreactors, and industry-based or municipal wastewaters, which can be used as water and nutrient sources. They are fast growing, and as algae can use CO2 as a carbon source, it also has the potential to be used to capture CO2 from, e.g. power plant flue gases. Micro algae produce lipids that can be used to produce biofuels (Aresta, Dibenedetto and Dumeignil, 2012).

2.2.4 Wastes and residues

Wastes and residues can be originated from different sectors. Municipal waste is trash or waste that is produced by households, construction sites and small business units. The biobased part of the waste is organic materials containing lipids, proteins and cellulose, e.g. food wastes, garden wastes, papers and used cooking oils (Sillanpää and Ncibi, 2017).

Animal-based waste lards, collected from slaughterhouses and livestock carcasses, can also be utilised in fuel production. This so-called technical grade brown lard is not suitable for food production or even animal feeding, and it needs to be pre-treated and cleaned before it is suitable for fuel production (Baladincz and Hancsók, 2015)

Pulp and paper mill wastes, like sludge and black liquor, food industry wastes and wastes from the vegetable oil industry are also potential biobased materials for further processing. Also, the agricultural sector leaves biomass waste as cereal plant straws, corn stoves and rice husks (Sillanpää and Ncibi, 2017)

3 Biofuels

A large share of CO2 emissions in the European Union are caused by the transportation sector, and the EU is also very dependable on imported oil. Biofuels are the primary means to reduce CO_2 emissions and increase energy independence (Energy Visions 2050).

European Renewable Energy Directive (RED) was introduced in 2009 to establish a policy for producing and using energy from renewable sources in the EU. Over the years, directives have been updated to speed up GHG emissions reduction. In 2023, RED III was published, raising the overall renewable energy target for the transportation sector for 2030 to 29% renewable energy or a 14.5% reduction in GHG intensity. RED III expands the overall target to all transport sectors, road, rail, maritime and aviation, as RED II calculated the percentage of road and rail fuels (ICCT).

The increasing demand for biobased fuels and chemicals can threat the overall GHG reductions if the raw material production is not done sustainably. Indirect land-use change can occur, e.g. if the biofuel production is started in areas that have been used for food or feed production leading to food vs. fuel dilemma negatively affecting food production. More effective methods are needed to feed the growing world population, and no arable land areas should be wasted on fuel production.

Besides setting the targets for renewable energy usage in the EU, the RED directive also aims for the sustainability of bioenergy production. It sets definitions for raw materials, like wastes and residues and measures indirect land use change (Mai-Moulin et al., 2021). The production of second and third-generation biofuels using feed materials like lignocellulosic materials, wastes, manure, sewage sludge and algae are promoted phasing out the first-generation biofuels. RED Article 17 sets sustainability criteria to protect biodiversity and prevent harmful indirect land use change. Raw materials should not come from areas that have been earlier peatland, primary forest, other high-carbon stocks, or highly biodiverse grasslands (Biograce).

3.1 Biomaterial conversion methods

Different methods are needed to transform the biomass into desired products depending on the biomass. The biomass feedstock can be divided into three classes: starchy feedstock, which includes sugars; triglyceride feedstock; and lignocellulosic biomass (Alonso, Bond and Dumesic, 2010). Figure 2 presents the chemical structure of biomass feedstocks.

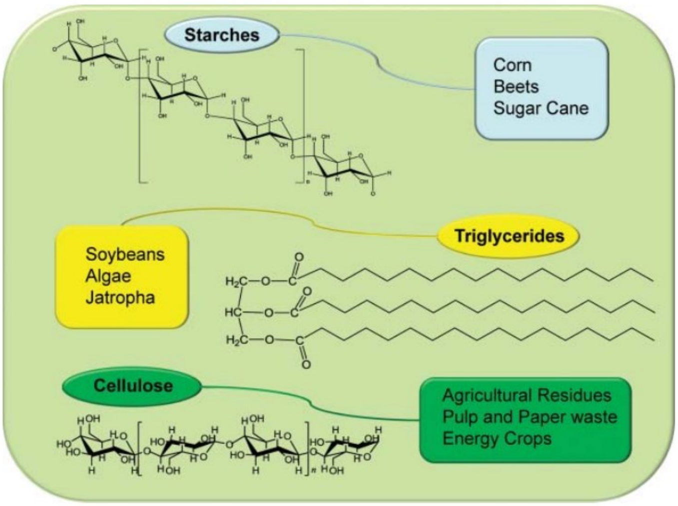


Figure 2 Biomass feedstocks chemical structure (Alonso et. al., 2010)

As the chemical structure varies, the complexity and process conditions of the biomass conversion methods also vary.

The first-generation bioethanol fermentation from sugarcane is a relatively simple process compared to, e.g. second-generation bioethanol production of lignocellulosic biomass as shown in Figure 3. The juice of sugarcane milling is readily fermentable sugars, mainly sucrose. After fermentation is the separation and purification of bioethanol using a distillation process. (Sillanpää and Ncibi, 2017).

The lignocellulosic biomass contains cellulose, hemicellulose and lignin. Cellulose and hemicellulose are polysaccharide polymers, and they are covered with a protecting layer of complex and recalcitrant lignin. The removal of ligning causes many technical challenges, and many process steps are needed before polysaccharides are depolymerised into fermentable sugars (Sillanpää and Ncibi, 2017).

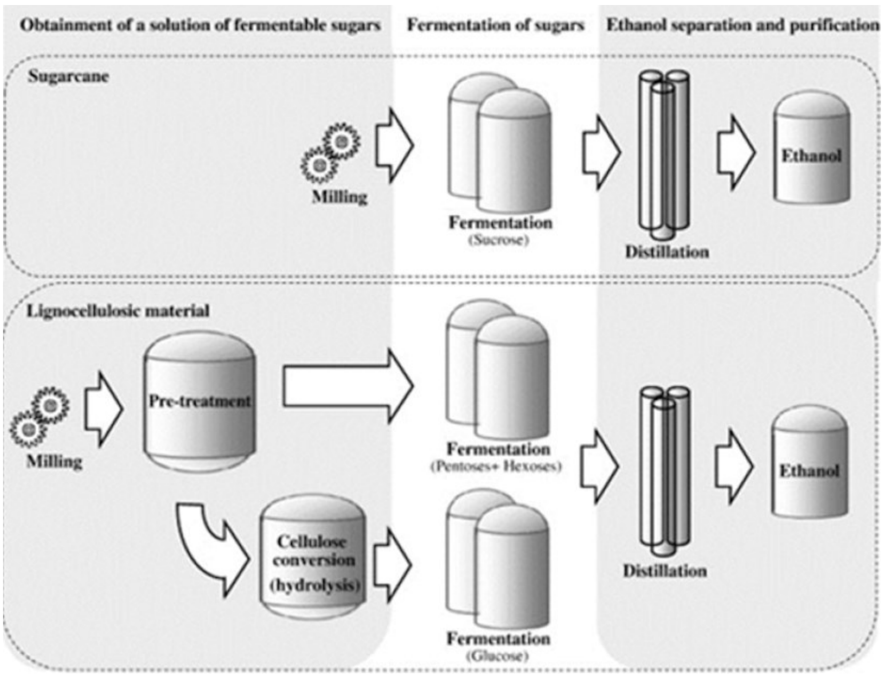


Figure 3 Bioethanol production from corn and lignocellulosic material (Sillanpää and Ncibi, 2017)

Comparing these two different bioethanol production processes leads to a dilemma related to food vs. fuel production. Ethanol production from sugar-containing biomass is easy and efficient, but it will threaten food production, and it is not sustainable. Bioethanol from lignocellulosic feed material is still mostly in the development phase, and the production costs are higher. As the availability of lignocellulosic raw material is almost endless, it is essential to continue to develop efficient methods to produce, e.g., bioethanol from it.

Fermentation is one method to produce biobased substances, but it is not suitable for all. Figure 4 presents different methods to convert biomass to fuels and the possible fuel that can be made after processing steps.

Biomass			
	Extraction		
		Transesterification	Biodiesel
	Hydrolysis		
		Fermentation	Biogas
			Ethanol
	Gasification		
		Synthesis gas	Biogas
			Hydrogen
			Methanol
			Ethanol
	Pyrolysis		Hydrogen
			Bio-oil
	Hydrotreating		Diesel

Figure 4 Different methods to convert biomass to fuels (Speight, 2020)

3.1.1 Extraction

Extraction method can be used to separate, e.g. juice, pulp, fermentable sugars or oils from the biomass. Mechanical extraction processes use pressure to press oil out from the kernels or seeds. Chemical extraction uses organic solvents to dissolve the oil from the material, and mechanical pretreatment is often needed for efficient solvent extraction. The enzymatic extraction process uses enzymes instead of solvents. The process is slower but more eco-friendly as no harmful solvents are needed (Sillanpää and Ncibi, 2017).

3.1.2 Hydrolysis

Hydrolysis is used to treat lignocellulosic or starch-containing biomass to release C5 and C6 monosaccharide sugars, which can be used to produce ethanol or other chemicals. Acid-catalysed hydrolysis uses sulfuric acid as a catalyst, and enzymatic hydrolysis uses different enzymes. Enzymatic hydrolysis is slower, but the operating conditions are milder than acid-catalysed. Efficient pre-treatment is needed to remove lignin as the enzymatic hydrolysis targets mainly the cellulose fraction (Sillanpää and Ncibi, 2017).

3.1.3 Gasification

Gasification is a thermal conversion system, where, e.g., solid biomass like dry wood chips, is partially converted into a gas mixture called synthesis gas, syngas. Using controlled oxygen level and temperature, part of the biomass is burned to provide heat for the gasification processes. Produced syngas is a mixture of CO, CO_2 and H_2, and it can be used as fuel or after cleaning processes, upgrade to chemicals, hydrogen or synthetic fuels (Speight, 2020).

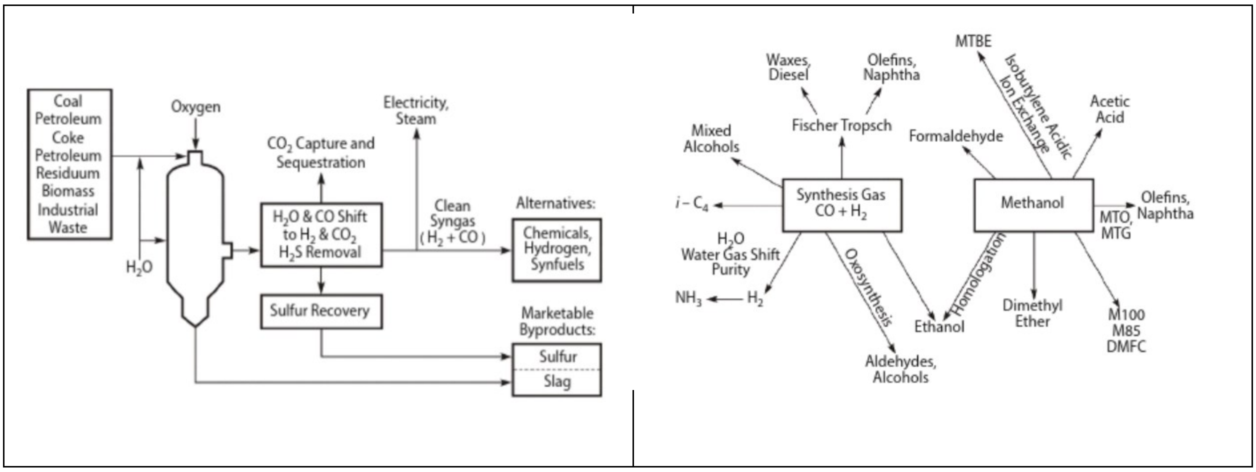


Figure 5 Gasification process and potential product from the syngas (Speight, 2020)

Figure 5 presents the gasification process. In the gas-cleanup process step, the CO2 captured and gas can be used as a fuel, e.g. in a powerplant gas turbine, or further processed to produce higher value products. Possible and potential products are in the Figure 5.

The feed can also be in the liquid phase, and one interesting biobased feed material is the by-product of the kraft pulp mill, black liquor. It consists of lignin and hemicellulose residues and inorganic chemicals used in the process (Speight, 2020). Nowadays it is mainly burned to produce energy in the plant but by using e.g. gasification technology it could be upgraded to higher value chemicals.

3.1.4 Pyrolysis

Pyrolysis is another thermal conversion process. Compared to gasification, where some level of oxygen is present, and part of the mass is burned, the pyrolysis process occurs in an oxygen-deficient environment. Pyrolysis is thermal decomposition of biomass, e.g., dry lignocellulosic materials or municipal solid waste (Samer and Mohamed, 2017).

Pyrolysis processes can be divided into two different processes depending on the speed of the process.

Fast pyrolysis occurs at 450-550°C temperature, and the residence time is short, 0.5-2 seconds. Fast heating and fast cooling aim to maximize the liquid product, bio-oil, yield. Bio-oil can be used as fuel in power plant boilers or upgraded to higher-value fuels or chemicals (Brown and Stevens, 2011).

The temperature range for slow pyrolysis is similar to fast pyrolysis, but the residence time is the main difference. With longer residence time, the main products are biochar and gases (Samer and Mohamed, 2017).

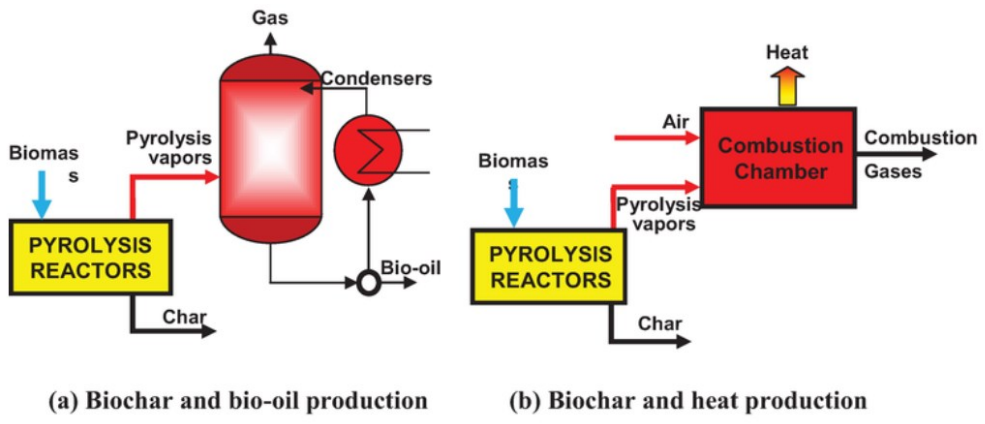


Figure 6 Fast and slow pyrolysis (Samer and Mohamed, 2017)

Fast pyrolysis process to produce bio-oil as the main product is in Figure 6a, and slow pyrolysis to produce biochar 6b.

3.1.5 Hydrotreating

Hydrotreating processes in the petroleum industry are used to remove unwanted contaminants like sulphur and nitrogen from petroleum to produce fuels. Hydrotreating processes occur in high pressure with hydrogen and a catalyst. In biofuel production hydrotreating processes can be used e.g., to remove the main contaminant, oxygen, from pyrolysis bio-oil (Brown and Stevens, 2011).

Producing high-quality renewable diesel or aviation fuels require also hydrotreating. Biomass originated oils and fats constitute usually of glyceride molecules like triglycerides and free fatty acids (Aslam et.al., 2022a).

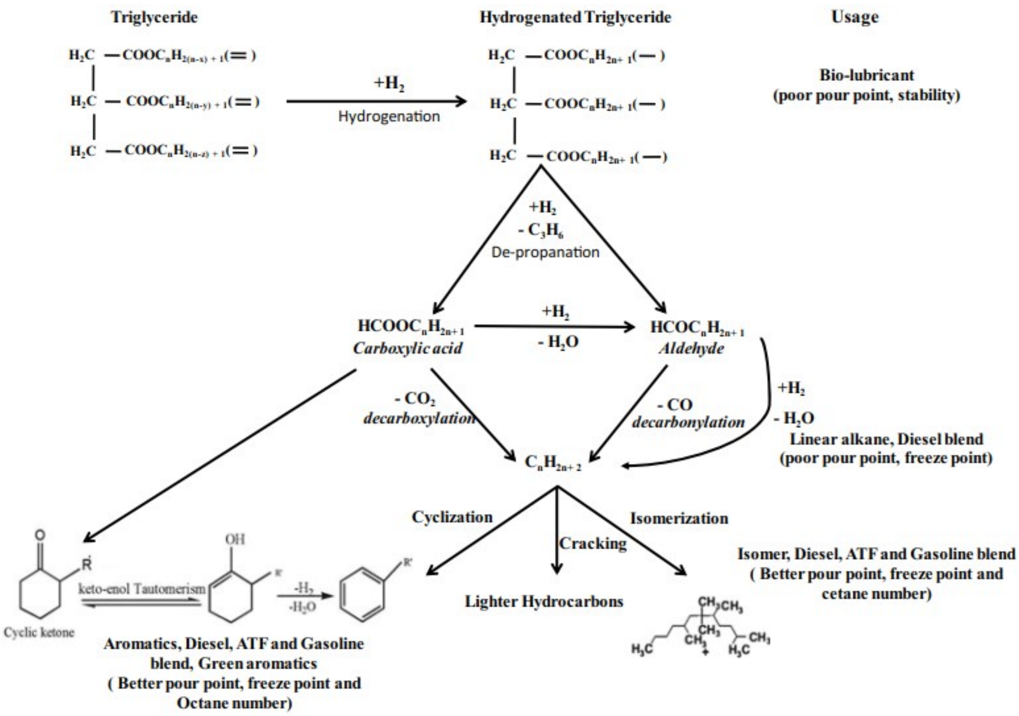


Figure 7 Reaction schemes for the hydroconversion of lipids into fuels (Aslam et. al., 2022a

Figure 7 presents the reaction schemes, hydrogenation of triglycerides, oxygen removal and isomerization process steps to produce high quality Hydrotreated Vegetable Oil (HVO) diesel fuel.

3.2 Biodiesel and HVO diesel

Conventional biodiesel which is manufactured by alcoholizing vegetable oils using simple alcohols such as methanol, ethanol or propanol and NaOH or KOH, produces fatty acid methyl ester (FAME) biodiesel. The main reactions are presented in Figure 8. (Aslam, Shivaji Maktedar and Sarma, 2022b).

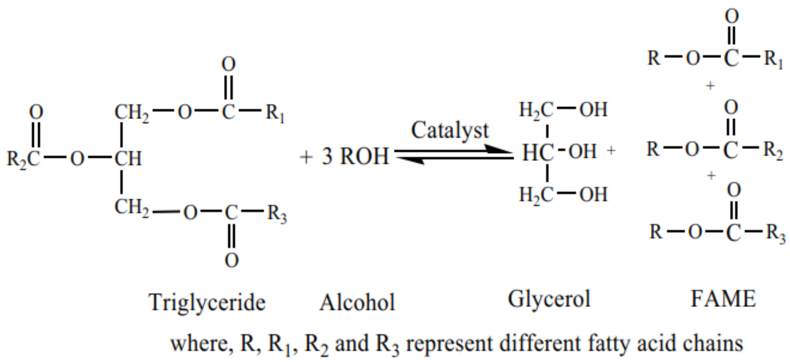


Figure 8 Schematic representation of biodiesel synthesis via transesterification (Aslam et. al. 2022b)

In common discussion, all biobased diesel fuels are often called biodiesels. Still, the big difference in quality, properties, and usage limitations between FAME and HVO diesel presented in Figure 7 requires that these should not be mixed. Table 1 presents the main properties of these fuels/fuel components. FAME can be used as a biocomponent in fuel, as there are maximum content limitations on how much it can be blended with fossil-based diesel fuel. FAME cannot be used as 100% fuel in modern diesel engines compared to HVO diesel, which can be mixed with fossil-based fuels without limitation or used as 100% fuel without any changes or modifications needed for the engine.

Table 1 FAME and HVO comparison (Aslam et. al. 2022b)

	FAME	HVO
Cold properties, cloud point	-5 °C	-34 °C (Neste My winter quality)
Oxygen content	11 %	0%
Max. blending with fossil-based diesel	7 %	100%
Storage stability	Marginal	Good

Poor FAME cold properties, instability during long-term storage and motor oil degradation if FAME content is high (Aslam et. al. 2022b) are a few main limitations to mention compared to HVO diesel.

3.3 Bioethanol

Bioethanol is an old and well-known biofuel produced largely as first-generation biofuel. Sugarcane and corn are used to produce bioethanol, but development towards the utilisation of second-generation raw materials is an important task. Using lignocellulosic biomass as feedstock would open almost unlimited raw material options, and if low-cost biomass residues could be used, the large-scale bioethanol production could be possible with competitive cost level (Gupta et al., 2014).

Ethanol can be mixed with gasoline up to 30% without engine modifications, or 85% mixture in specially designed engines.

4 Oil refinery co-processing

The interest in biofuel production in traditional oil refineries is currently growing. The oil refineries have well-developed infrastructure to produce, store and distribute fuels and chemicals, which reduces the costs compared to a new stand-alone biofuel production plant.

OPEX and CAPEX costs are reduced as there is no need to establish parallel systems (Bezergianni, Dimitriadis, Kikhtyanin, and Kubička, 2018). Also, modification of old process unit for co-processing can be beneficial and payback time short, if e.g. metallurgy of the process unit is suitable for biobased components. Marker (2005) estimated the possibility of reducing investment requirements by 50% or more when retrofitting existing process units like MTBE or MEROX in biofuel production.

Co-processing, feeding mixture of bio-based feedstock and petroleum fractions produces low-carbon hybrid fuel, partially bio-and partially fossil-origin. The main process units for co-processing are fluid catalytic cracking (FCC) and catalytic hydroprocessing units. (Bezergianni et al., 2018). Differences between stand-alone biobased feedstock hydroprocessing units and co-processing in petroleum oil refineries are shown in Figure 9.

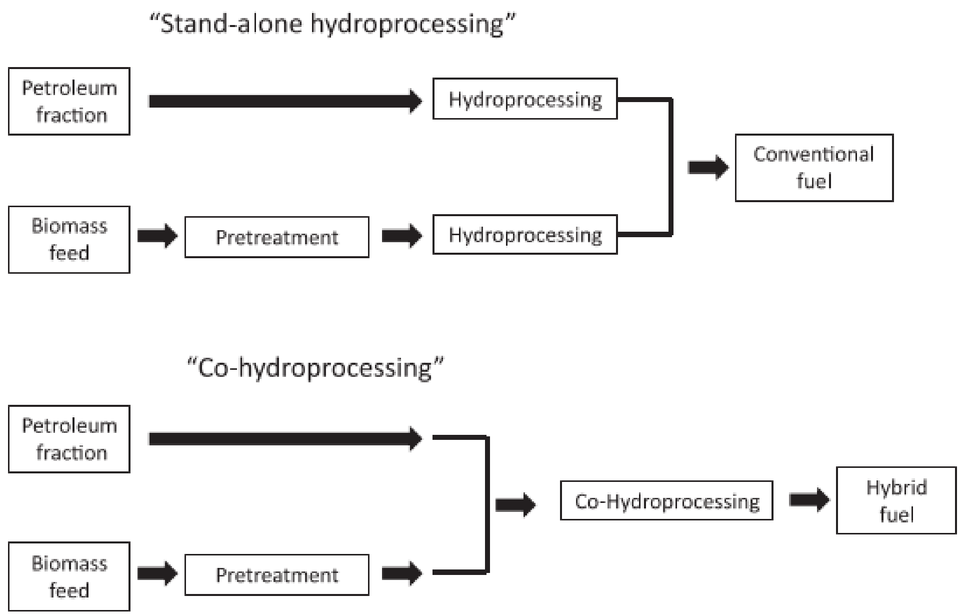


Figure 9 Stand-alone biomass hydroprocessing unit producing drop-in biofuel and co-processing (Bezergianni et al., 2018)

Stand-alone hydroprocessing unit produces drop-in biofuel mixed with hydroprocessed petroleum fraction. The combined product is conventional fuel with a biocomponent. Co-processing in the hydroprocessing unit processes the petroleum fraction and pre-treated biobased feed simultaneously, and the product is a hybrid fuel.

Besides existing infrastructure, co-processing bio-based feed at existing petroleum refineries with petroleum fractions can also be beneficial as it can allow the refineries to meet national biofuel mandates (Bezergianni et al., 2018).

4.1 Biomass-derived feedstock for co-processing

Several different biomass-derived could be used as feed material in co-processing. Waste cooking oils, non-edible oils, animal fats and bio-oils, e.g. from pyrolysis or liquefaction, are suitable feed materials, and they can be co-processed with petroleum fractions in FCC or hydroprocessing units (Bezergianni et al., 2018).

Biomass-derived feedstock composition varies based on the source and pretreatment method used. Table 2 presents different feedstock alternatives and their main composition compared to Vacuum Gas Oil (VGO). VGO is one possible petroleum fraction, that could be used in co-processing (Bezergianni et al., 2018) feeding the process unit with a mixture of VGO and biobased feed material.

The composition of biomass-derived feed material varies largely based on the biomass type and pre-treating process. For example, with the pyrolysis process, it is possible to produce bio-oil, which can be used as heating oil in power plants (Green Fuel Nordic). GFN bio-oil water content is 21 w-%, and the lower heating value is 18.2 MJ/kg. Compared to wood-based fuels or biomasses, it is easier to transport and store, but to produce standards meeting traffic fuels, bio-oil needs more quality upgrading. After oxygen removal, pyrolysis bio-oil could be processed, e.g. in FCC units, to produce fuels and gases (Mercader, Groeneveld, Kersten, Way, Schaverien and Hogendoorn, 2010).

Table 2 Pyrolysis oil, biobased lipids and petroleum VGO properties (Al-Attas, Lucky and Hossain (2021); Mercader et al. (2010); Bezergianni et al. (2018))

	Pyrolysis oil, Forest residue	Palm oil	Rapeseed oil	Waste lard	VGO
Oxygen [w-%]	45-50	11.33	10.6	10.5	0.094
Sulfur	0.01 w-%	100 ppm	100 ppm	270 ppm	2.98 w-%
Nitrogen	0.2 w-%	1.6 ppm	16 ppm	232 ppm	0.95 w-%

In general, petroleum has a high content of hydrocarbons with almost no oxygen compared to biomass-derived feed which has high oxygen content and a smaller number of hydrocarbons (Sillanpää and Ncibi, 2017). Bio crude oil from pyrolysis has the highest oxygen content, orientated from the decomposition of lignin, hemi-cellulose and cellulose and the remaining moisture from the raw material (Bezergianni and Dimitriadis, 2013).

4.2 FCC

The fluidized catalytic cracking unit (FCC) is one of the most important units in petroleum refineries. FCC can crack heavy low value petroleum streams to produce higher-value products like gasoline, C3/C4 olefins and LPG. Gasoline is the main product in a typical FCC unit, but some FCC units are designed for the production of petrochemicals (Fahim, Alsahhaf and Elkilani, 2010).

A generic presentation of an FCC unit is shown in Figure 10. Heated feed and steam are fed to the bottom of the riser, where they mix with hot catalyst and go upwards to the reactor section. The riser pipe is a long vertical pipe, and it is the actual reactor, where endothermic reactions take place. The produced gaseous products and heavier liquid hydrocarbons, which are stripped from the catalyst with stripper steam, go to the fractionator for further separation.

The used catalyst is highly active zeolite based catalyst (Venuto and Habib Jr, 1979). The activity of the catalyst falls in the process because of the fast coke formation over the catalyst surface. The spent catalyst flows from the reactor to the regenerator, where the formed coke is burned with excess air. Coke burning regenerates the catalyst, and the heated catalyst flows back to the riser. There is a heat balance in riser/regenerator system, all the heat needed to vaporize the feed and needed for the endothermic cracking reactions is formed in the regenerator when the coke is burned (den Hollander, Makkee and Moulijn, 1998).

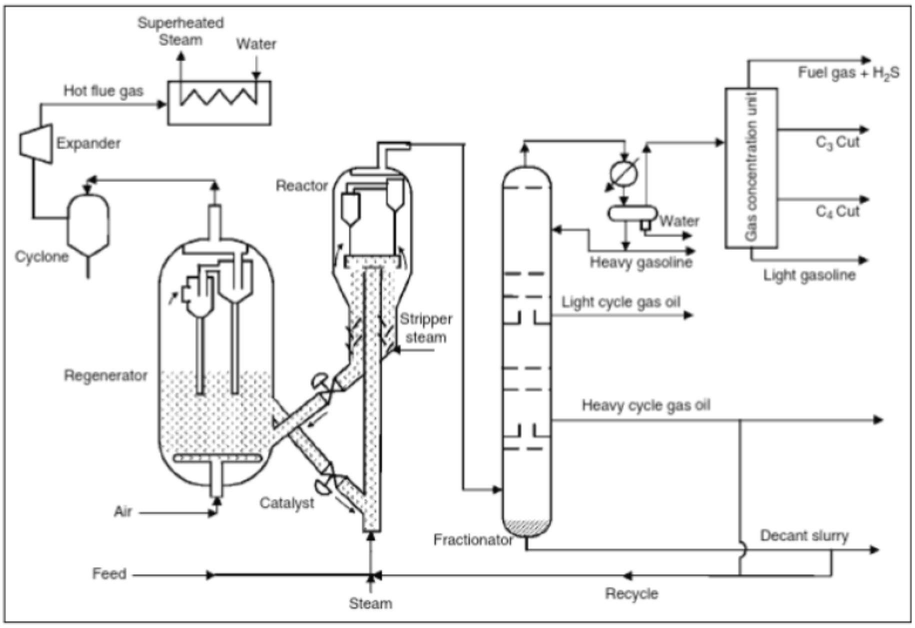


Figure 10 Typical side-by-side FCC unit (Fahim et. al. 2010)

The main FCC unit feed is gas oil and heavy gas oil streams with boiling points between 316-566 °C containing aromatic, naphthenic, olefinic and paraffinic molecules. As the higher boiling point fractions can have a high number of contaminants like sulphur, nitrogen and metals, the feed needs to be hydrotreated before it can be fed to the FCC. (Fahim et. al., 2010). As there is no sulphur removal in FCC, the sulphur content in feed separates into products, and producing, e.g. gasoline, which has a maximum limit for sulphur, the feed sulphur level must be low enough to meet this limitation. Metals, most commonly nickel and vanadium, act as catalyst poisons, as they block catalyst active sites, so metals should be removed in the feed pre-treating unit. Nitrogen acts as a temporary catalyst poison on the catalyst surface as it can neutralise acid sites, but the process should not be affected if the nitrogen level is controlled below 0.2 % (Fahim et. al., 2010). Also feed oil coke formation tendency can limit the feed rate if the coke formation is too high compared to the burning capacity. Conradson carbon residue (CCR) is laboratory test which indicates the thermal coke formation tendencies of an oil (den Hollander, Makkee and Moulijn, 1998).

4.2.1 FCC Co-processing

FCC is potential processing unit for co-processing, as it requires no additional hydrogen (Repsol) and the reactor conditions are enough severe to decompose the oxygenated hydrocarbons (Bezergianni et al., 2018). Also, the continuous catalyst coke removal in regenerator maintains the catalyst activity.

One possible renewable feed source is bio-oil, that can be produced e.g. with pyrolysis technology from lignocellulosic biomass. The basically infinite lignocellulosic biomass is low-cost energy source, and with further upgrading processes bio-oil could be used to produce chemicals and traffic fuels.

Pyrolysis bio-oil has many adverse properties, like high content of reactive oxygenates causing instability, low heating value and corrosivity. Bio-oil is also immiscibility with hydrocarbon fuels and contains relatively large amount of water. These unwanted properties have limited the bio-oil usage in energy market (Stefanidis, S. D., Kalogiannis and Lappas, 2018), and further quality upgrading is needed to increase bio-oil usage. Test runs with laboratory and pilot scale equipment with different bio-oil/petroleum-based feed have been done, and with suitable ratio have the results been promising.

Previous studies (Vitolo et al., 1999); (Adjaye, Katikaneni and Bakhshi, 1996) has shown that pure bio-oil processing causes high yields of char, coke and tar leading to low hydrocarbon yields and other severe operation issues, but several co-processing tests with laboratory and pilot scale equipment has shown, that with sufficient feed ratio, the processing is possible against the limitations that the co-processing causes. Coke formation will increase, and de-oxygenation reactions causes increased formation of CO, CO_2 and H_2O (Stefanidis et. al. 2018). As some research consider high bio-oil content in feed, up to 20 w-% that could be co-processed with VGO, more realistic content could be in the range 5-10 w-% (Bertero and Sedran, 2015).

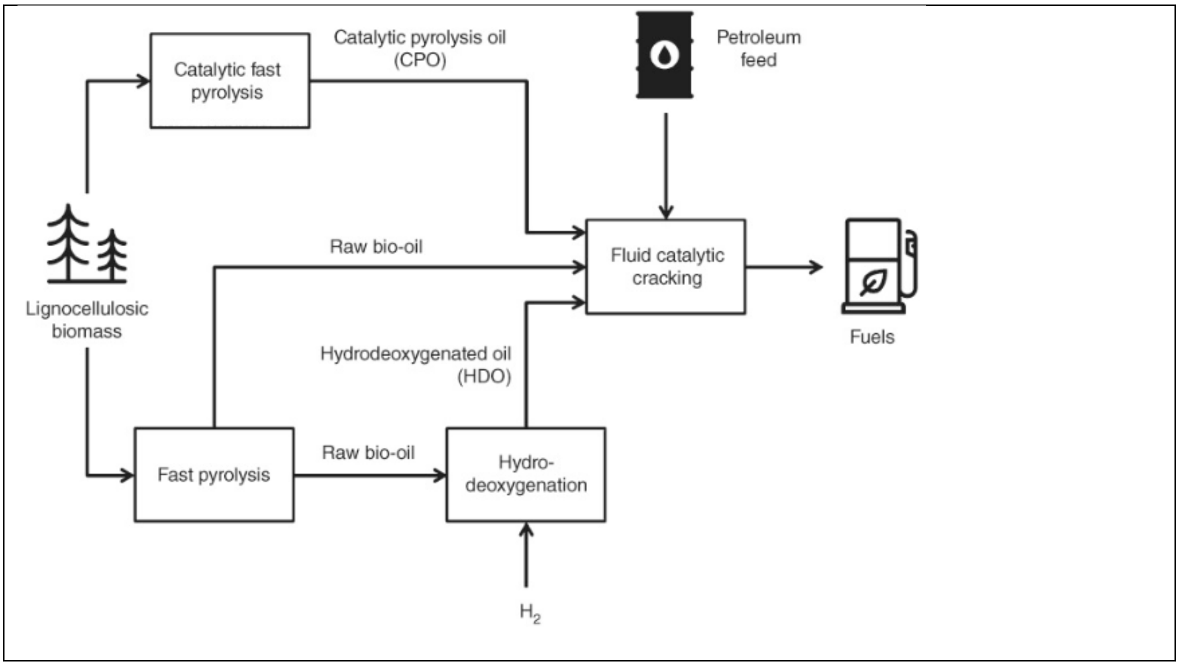


Figure 11 Pyrolysis feed routes for FCC (Stefanidis et.al. 2018)

Different possible routes for different pyrolysis oils for FCC feed are shown in Figure 11. Fast pyrolysis bio-oil requires pre-treating, oxygen removal, before it can be fed to FCC unit. The quality of bio-oil from catalytic fast pyrolysis is higher, and additional pretreatment is not necessary.

4.3 Catalytic hydroprocessing

Catalytic hydroprocessing consist of two technologies, hydrocracking (HDC) and hydrotreating (HDT). Hydrocracking process produces lighter, lower boiling point products from heavier feedstock and hydrotreating process aims to remove undesirable substances like sulphur, nitrogen, oxygen, metals and partial oxygenation of aromatics hydrocarbons (Bezergianni et al., 2018). Desired reactions are enabled with addition of hydrogen in presence of catalyst.

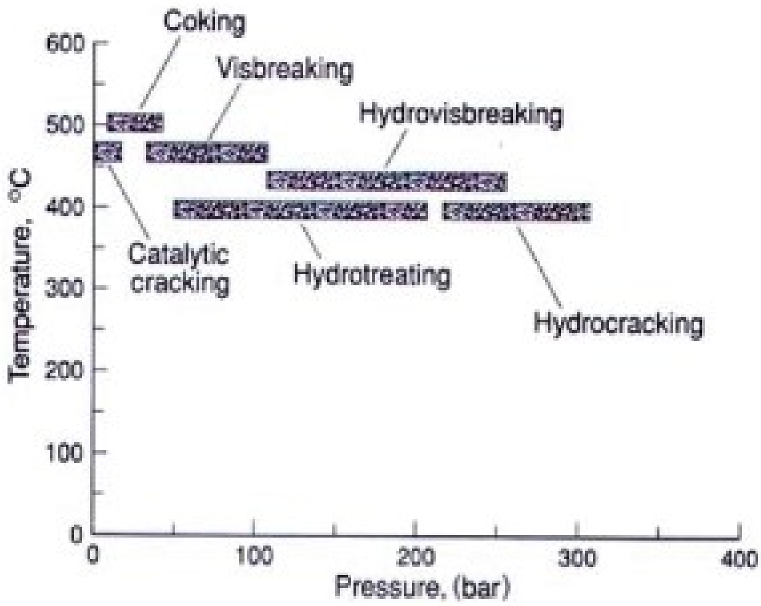


Figure 12 Temperature and pressure parameters for various petroleum refinery processes (Speight, 2020)

Figure 12 shows different petroleum refinery processes pressure and temperatures, including catalytic cracking (FCC), hydrocracking and hydrotreating processes. From these, the process severity is highest in hydrocracking processes, as it has the highest hydrogen partial pressure, and the feed has a longer residence time in the reactor. Hydrocracking is destructive hydrogenation as the purpose is to convert higher molecule-weight hydrocarbons to lower boiling point products. This requires high hydrogen pressure to avoid coke formation and to minimize polymerization.

4.3.1 Hydrotreating

Hydrotreating can be considered as non-destructive hydrogenation, and it has milder conditions as the purpose is to attack only the undesired components, not to change much the boiling range. (Speight, 2020) Main reactions include hydrodesulphurization (HDS), hydrodenitrogenation (HDN), hydrogenation (HYD), hydrometallization (HDM) and hydrodeoxygenation (HDO) (Bezergianni et al., 2018).

For example, the removal of sulphur from fuels is important to reduce SOx emissions, and the removal of nitrogen reduces NO_x emissions. HDM reactions are important to protect downstream catalysts, and HDN and HDS reactions can also be important for the same purpose. HYD reactions saturate feedstock and can e.g. reduce aromatic components and HDO reactions remove oxygen which is unwanted component in some of the fuels (Bezergianni et al., 2018).

4.3.2 Oxygen removal

Considering the co-processing of biobased feed, the oxygen removal is essential as the biomass contains oxygen much more than fossil hydrocarbons. As shown in Table 1, pyrolysis oil contains oxygen 45-50 w-%, vegetable oils 10-11 w-% and waste lard 11-w% compared to fossil petroleum distillate VGO which contains 0.09 w-% oxygen.

Reaction pathways and stoichiometry off hydroprocessing triglycerides are shown in Figure 13.

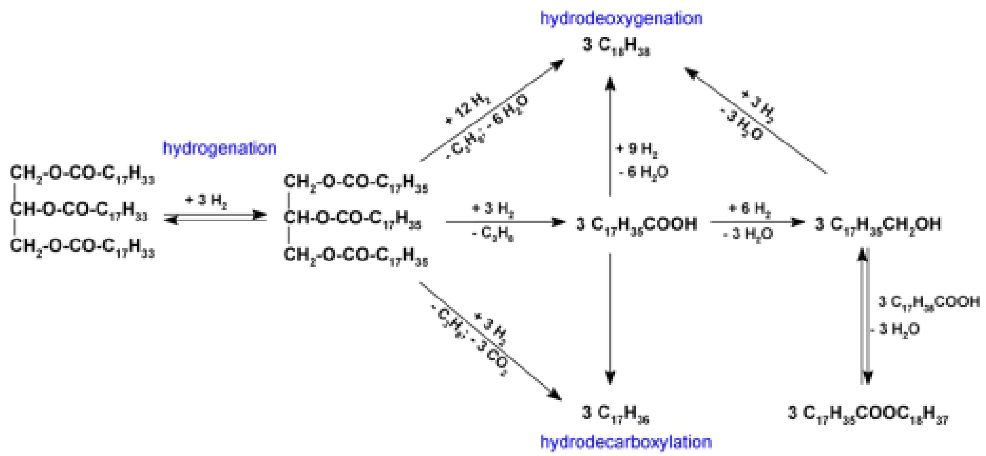


Figure 13 Reaction stoichiometry and pathways of hydroprocessing triglycerides (Chen, Farooqi and Fairbridge, 2013)

The processing of triglycerides has two main pathways, hydrodeoxygenation (HDO) and hydrodecarboxylation:

In the HDO pathway one triglyceride molecule consumes 12 hydrogen molecules to form 3 normal hydrocarbons, e.g. n-octadecane (n-C18-H38).

In the hydrodecarboxylation pathway one triglyceride molecule consumes three hydrogen molecules to form 3 normal hydrocarbons, e.g. n-heptadecane (n-C17-H36)

Main products are typically hydrocarbons (n-alkans) which are suitable for diesel fuel production and by-products propane, CO, CO_2, and water (Bezergianni et al., 2018).

Figure 14 shows the HDO reactivity and hydrogen consumption of different oxygenates.

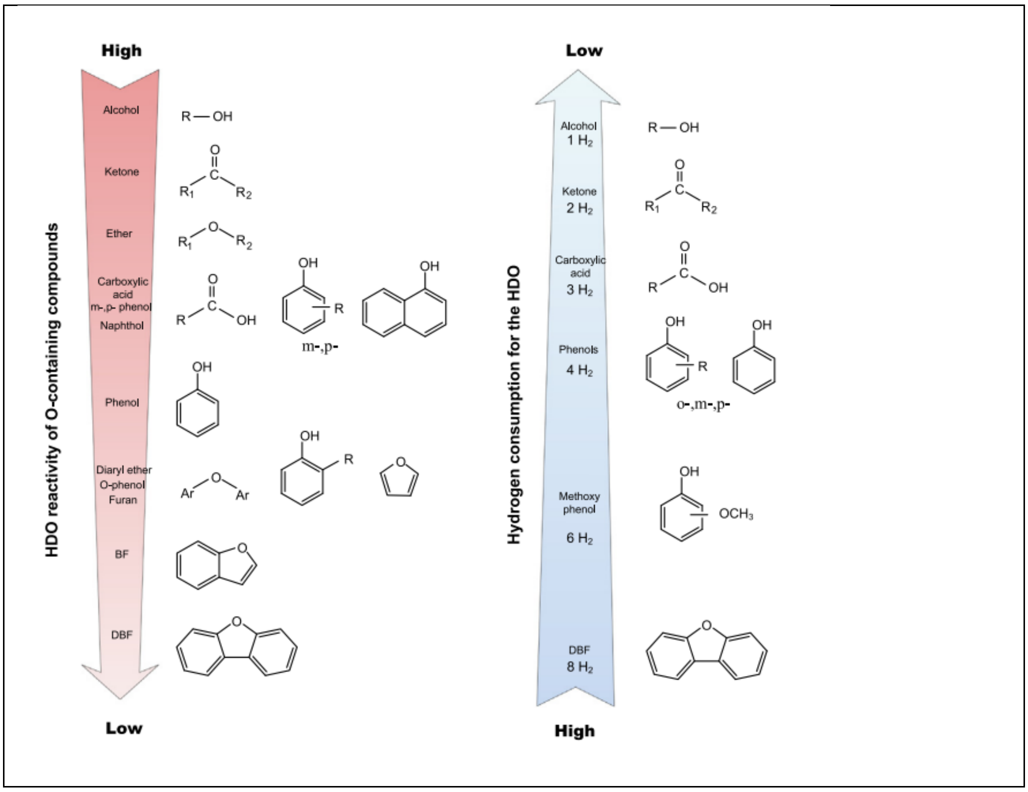


Figure 14 HDO reactivity and hydrogen consumption (Jensen, Hoffmann and Rosendahl, 2016)

The oxygenate content of biobased feed varies depending on the feed material source.

The main reaction classes that Corma et al. (2007) have proposed that are the HDO reaction pathways in the FCC process are:

- dehydration reactions
- cracking of large oxygenated molecules into smaller molecules
- hydrogen producing reactions
- hydrogen consuming reactions
- production of larger molecules by C-C bond-forming reactions

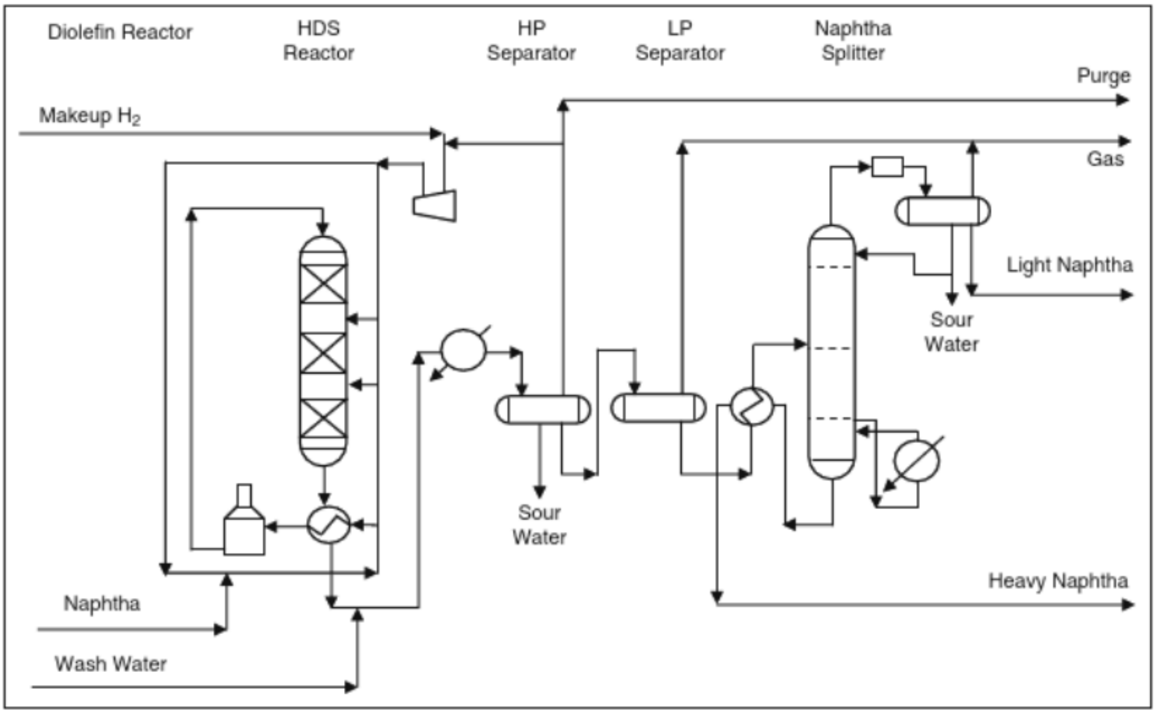


Figure 15 Naphta hydrotreating process (Fahim, Alsahhaf and Elkilani, 2010)

Figure 15 shows the basic naphtha hydrotreating process unit. Feed and recycle gas (mainly hydrogen) from the recycle gas compressor are heated in the furnace before entering the reactor from the top. The reactor has 3 catalyst beds, and part of recycle gas goes between catalyst beds to reduce the temperature after exothermic reactions. After the reactor stream temperature is lowered and two gas/liquid separators separate the liquid stream to product separation distillation and the gas stream back to the recycle gas compressor. Part of the gas is purged out from the loop to maintain gas purity, and make-up hydrogen is added to replace the hydrogen consumed in reactions and losses to the purging stream.

4.4 Co-processing production effects

Possible adverse effects from co-processing biobased feed depends by the biobased feed, refinery process, and the bio feed proportion of the total feed.

In hydrotreating co-processing processes, oxygen content leads to limitations that can be caused by oxygen removal reactions, as they compete in the reactor with other relevant reactions like sulphur removal. This can set maximum bio content limitation in the feed so that all product specifications are fulfilled (Bezergianni et al., 2018). HDO reactions also increase hydrogen consumption, which can also be a constraint in a refinery process unit setting the maximum limit for the bio feed. Increasing hydrogen consumption increases costs, and equipment-related constraints like gas compressor capacity can start to limit.

Bezergianni et al. (2014) studied co-processing of used cooking oil (UCO) with Heavy Atmospheric Gas Oil (HGO) with different ratios in laboratory scale hydroprocessing plant.

Figure 16 present their hydrogen consumption results from the test runs, that were performed at 350 °C temperature and 55 bar pressure. With 5-10% UCO content of the feed the hydrogen consumption increased by only 6.25%, so at least 10% feed content can be achieved without significant chance in operations cost related to hydrogen.

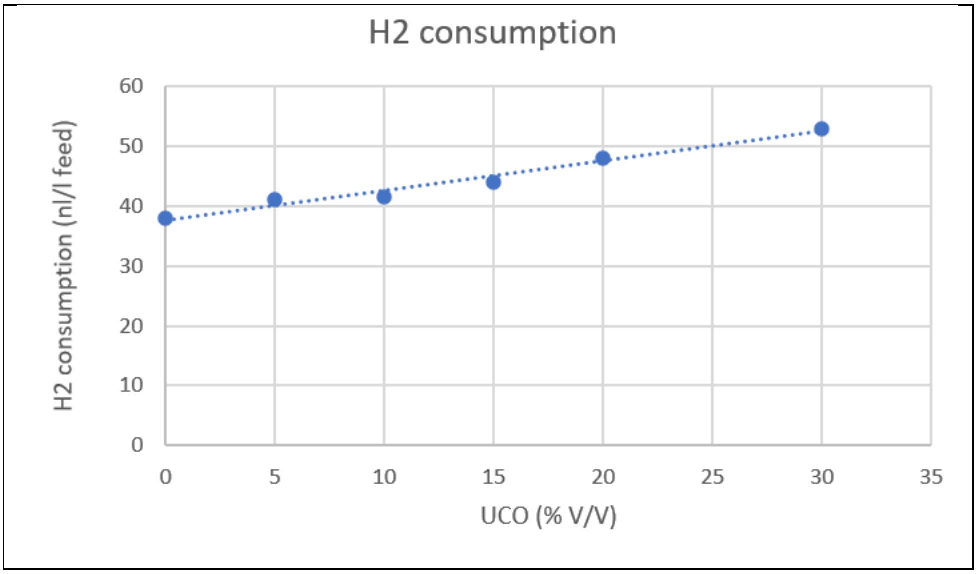


Figure 16 Hydrogen consumption in UCO/HGO test runs, modified (Bezergianni et.al., 2014)

Their study results also showed increasing diesel yield, so the conversion of middle distillate (sample boiling range 180-360 °C) distillate was increased, indicating that vegetable oil content in the feed can increase the conversion towards lighter products. Triglycerides are converted into normal C15-C18 molecules that are suitable for diesel fraction.

Reactor temperature affects yields, and higher reactor temperatures lead to more cracking reactions leading to an increase in lighter unwanted non gas oil fractions. Tóth, Baladincz, Kovács and Hancsók (2011) studied vegetable oil co-processing with gas oil. The reactor temperature effect on organic liquid phase yield is presented in Figure 17. Unwanted byproducts that are formed are CO, CO_2, H_2O and C_3H_8. The sulphur content of the product decreased, mainly as the vegetable oil sulphur content was low. After 25% vegetable oil content in the feed, the sulphur level in the product started to increase. This is caused by the deoxygenation reactions that are competing with the sulphur removal reactions.

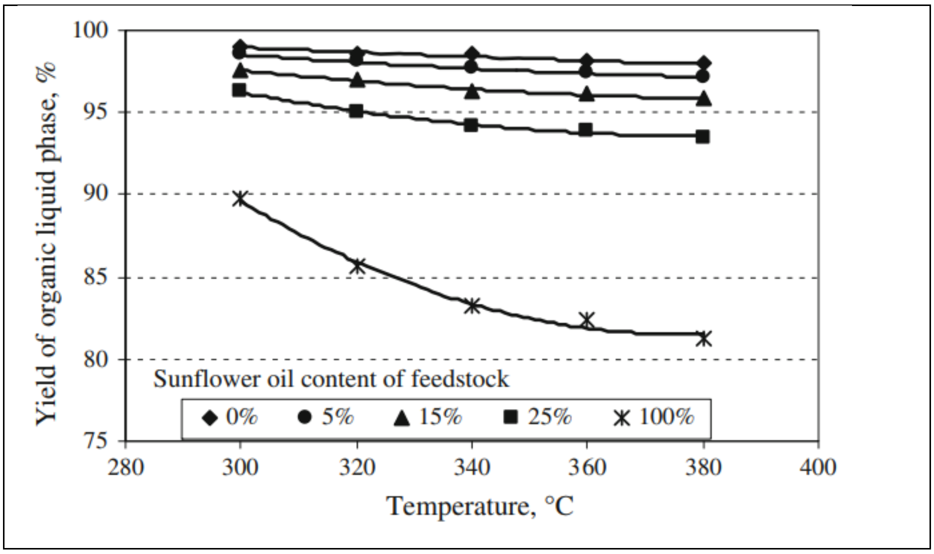


Figure 17 Organic liquid phased yield (Tóth et al., 2011)

Important product quality related to middle distillates, mainly diesel fuel, are the cold properties in winter grades. Cold filter plugging point, (CFPP), is the lowest temperature at which fuel can be used without the risk of clogging the fuel filter (Neste).

Conversion of triglycerides into normal paraffins is presented in Figure 13. These paraffins increase the cetane number of the fuel, but they have a negative effect on cold properties. This can limit the maximum bio component feed amount, at least in some product qualities.

One solution for better middle distillate cold properties is two-stage hydroprocessing. Baladincz and Hancsók (2015) studied waste animal fat co-processing with gas oil. The two-stage reactor setup had NiMo catalyst for hydrotreating in the upper part of the reactor, and Pt/SAPO-11 isomerisation catalyst on the bottom. After the hydrotreating step the CFPP was +8 °C and after isomerisation step -15-20 °C

5 Fixed bed reactors

The most common reactor type in petroleum refining is high-pressure trickle-bed reactor (TBR). This chapter presents the general reactor structure, the catalysts used, and how the reactor temperature is controlled.

5.1 Trickle bed reactor

Trickle-bed reactors are the most common three-phase reactor type used in industrial applications. In hydrotreating processes, the phases are hydrogen gas, liquid hydrocarbon feed and solid catalyst particles in the reactor. A TBR reactor consists of one or several fixed catalyst beds, and the feed, gas and liquid, is fed to the top of the reactor. The gas and liquid flow downwards in the reactor carrying both reactants and products, and nearly plug flow is achieved (Al-Dahhan, Larachi, Dudukovic and Laurent, 1997).

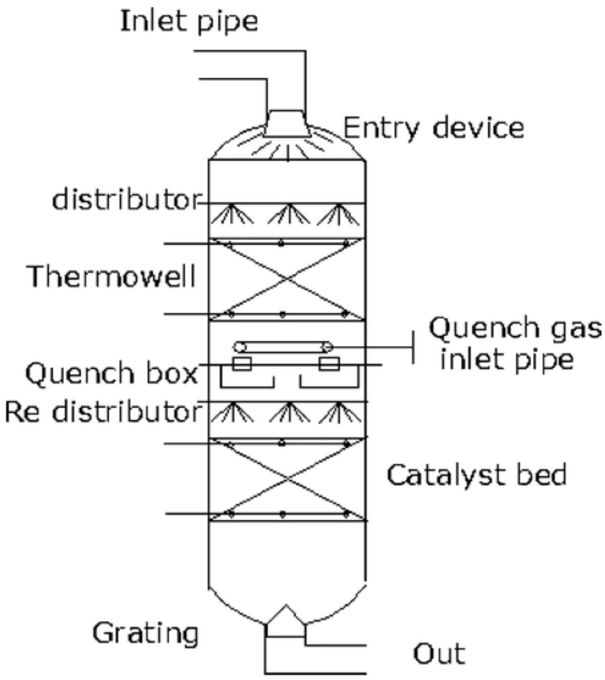


Figure 18 Schematic drawing of a trickle-bed reactor (Maiti and Nigam, 2007)

The drawing of a trickle-bed reactor (Figure 18) presents the main components of a TBR reactor. The TBR reactors are often used in high temperatures and pressures, and the reactions, like hydrogenation of unsaturated hydrocarbons, are strongly exothermic. Proper distribution of dissolved gas and liquid is done using distributors before the catalyst bed, and it is important to prevent liquid maldistribution in the catalyst, which can lead to local catalyst hotspot (Al-Dahhan et al., 1997). Temperature measurements in catalyst beds and hydrogen-rich recycle gas as quench between the beds are used to control the catalyst bed temperature.

5.2 Catalyst

Common catalysts used in petroleum hydrotreating consist of two parts: the support material and the active element. Support material has high porosity, which increases the catalyst surface area. Cobalt-Molybdenum (CoMo) for HDS and Nickel-Molybdenum (NiMo) for HDN on alumina (Al_2O_3) support are the most commonly used catalysts in hydrotreating (Stefanidis, S. D., Kalogiannis and Lappas, 2018). Reactor catalyst loading consist often of several different catalyst layers, and the loading is tailored based on the process conditions, feed quality, product target quality, etc.

5.3 Weighted average bed temperature

Weighted average bed temperature, WABT, is one key process variable related to hydrotreating reactors. It is a measured variable that can be used to follow catalyst deactivation and to set operation conditions so that the required catalyst activity is reached (Hsu and Robinson, 2006). Reactor temperature needs to be gradually increased, e.g., as the catalyst deactivates to hold e.g. the same sulphur removal efficiency.

The hydroprocessing reactions are exothermic so that the temperature will increase in the catalyst bed as the reaction products, oil and gas flow through the bed. The temperature increase is not linear in the catalyst bed (Ancheyta and Speight, 2007), as the fastest and easiest reactions occur at the beginning of the bed. Simple average calculation based on inlet and outlet temperatures of the reactor is not accurate to present the whole reactor temperature, so more temperature measurements are needed to calculate a better representation of process conditions. The temperature in the inlet and outlet of each catalyst bed is required, and several measurement points are needed to observe the temperature distribution radially. The average or median of these radial measurements can be used as the inlet or outlet temperature.

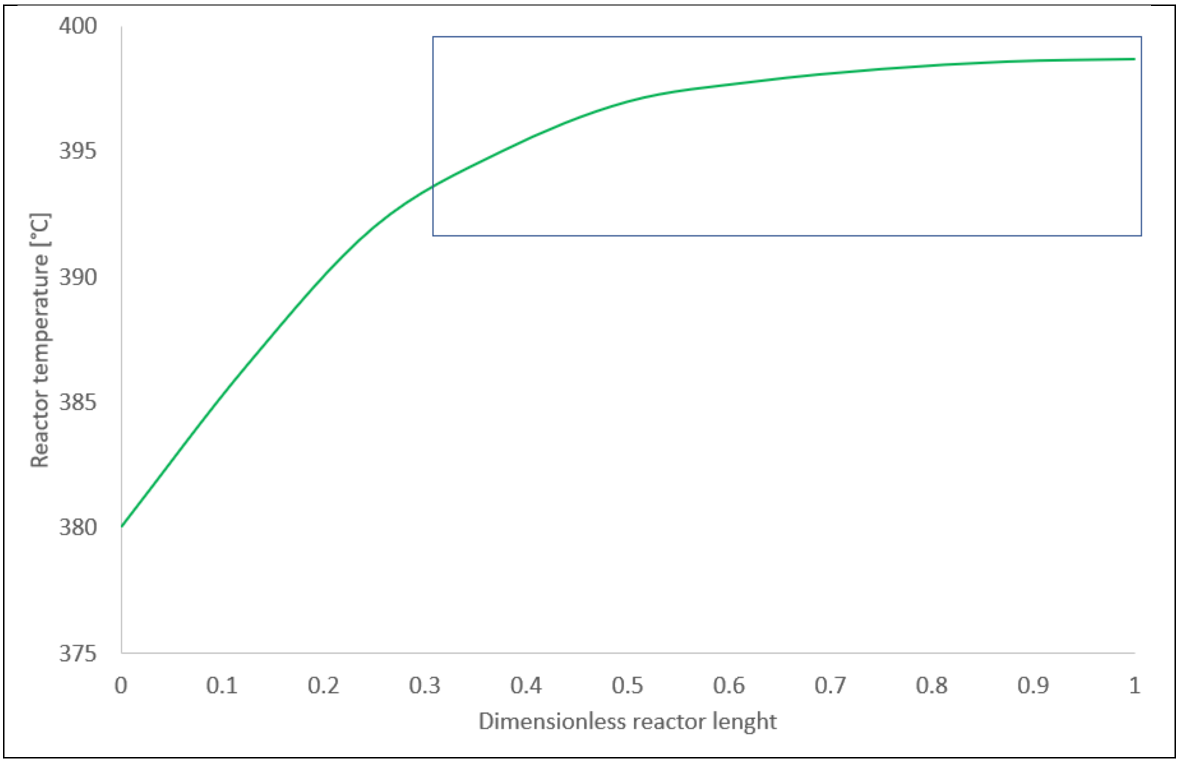


Figure 19 Example of reactor temperature profile (Ancheyta and Speight, 2007, modified). In the blue rectangle, the last 2/3 of the reactor length

Weighted average catalyst temperature is often calculated with the following equations (Ancheyta and Speight, 2007); (Stefanidis, G. D., Bellos and Papayannakos, 2005):

$$WABT_i = \frac{Tin + 2Tout}{3} \tag{1}$$

Where, Tin = Catalyst bed inlet temperature

Tout = Catalyst bed outlet temperature

$$WABT\ global \sum_{i=1}^{N} (WABT_i)(W_c\%) \tag{2}$$

Where, N= number of catalyst beds

Wc% = weight percent of catalyst in each bed

$$WABT_i = \frac{Tin + Tout}{2} \tag{3}$$

Equation 1 is used to calculate the average WABT of each catalyst bed or single-bed reactor. It takes into consideration the nonlinear temperature increment (Figure 20); last 2/3 of the catalyst is closer to the outlet temperature, and the first 1/3 is closer to the inlet temperature.

The global WABT for the whole reactor, if the reactor has more than one catalyst bed, is calculated using Equation 2.

Equation 3 can also be used for simple, rapid calculations, but it induces more error than equation 1 (Ancheyta and Speight, 2007).

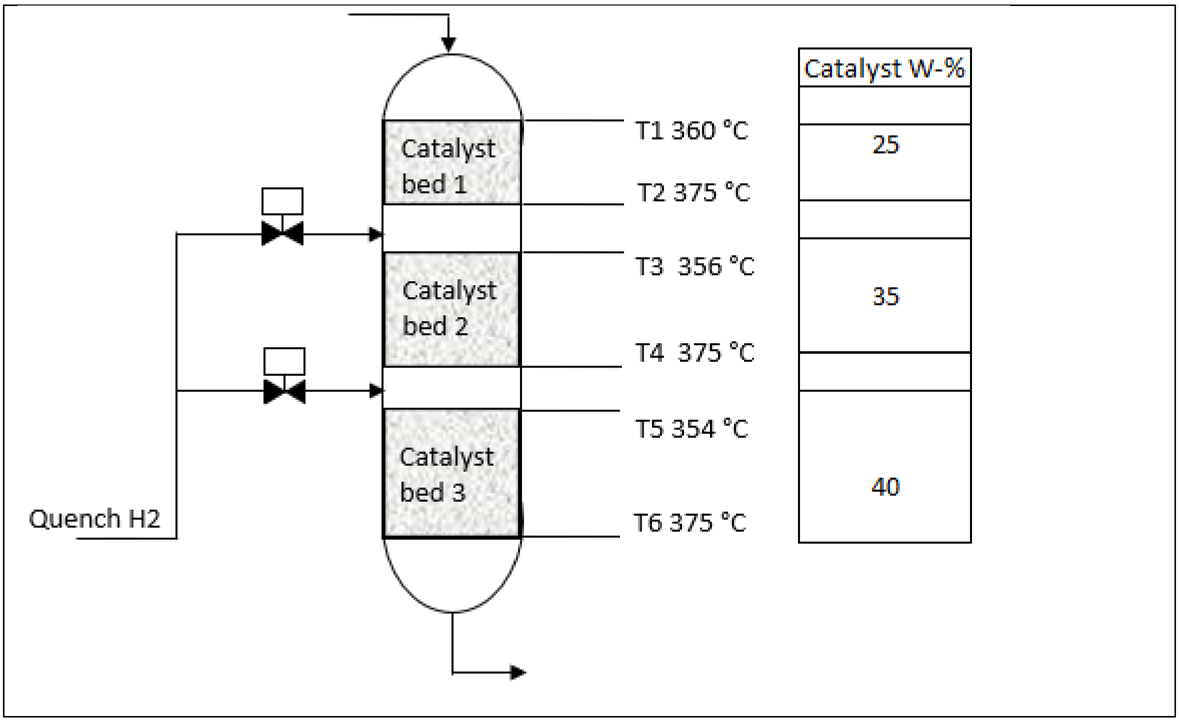


Figure 20 Example reactor

Figure 20 presents an example reactor, which has three catalyst beds. The first bed contains 25%, the second 35% and the third 40% of the total catalyst mass. Catalyst beds have temperature measurements on the top and bottom of each bed.

Comparing WABT calculations using Equations 1 and 3 and the results are presented in the table below.

Table 3 WABT calculations

	Equation 1	Equation 3
Bed 1	(360°C+2*375°C)/3*0.25	(360°C+375°C)/2*0.25
Bed 2	(356°C+2*375°C)/3*0.35	(356°C+375°C)/2*0.35
Bed 3	(354°C+2*375°C)/3*0.4	(354°C+375°C)/2*0.4
Global WABT (Eq 2)	Σ =368.7 °C	Σ =365.6 °C

Calculating the global reactor WABT using bed average temperature (Equation 3) underestimates the temperature compared to eq.1, where the outlet temperature has more weight. Table 3 shows the calculations and results.

5.4 Temperature control

High sulphur, nitrogen or olefin content in feed can cause over a 100 °C temperature increase in the reactor, so the catalyst is divided into multiple catalyst beds with cooling zones between the beds to decrease the temperature rise (ΔT) in one bed (Hsu and Robinson, 2006). Proper temperature control and monitoring of ΔT is important, and the risks increase with high-activity catalysts, mainly in hydrocracking processes. If more heat is generated than is possible to remove with flowing streams, there is a risk of temperature runaway. The speed of reactions increases when temperature increases, resulting in more generated heat, which can result in extremely high temperatures in a short period of time. These high temperatures can damage the catalyst and reactor (Treese, Jones and Pujado, 2020).

In trickle-bed units cooling is commonly done with recycle gas from the recycle gas compressor. Recycle gas is a gas stream mainly containing hydrogen, and besides the gas quenches, it is mixed with the oil feed before the reactor. Figure 21 presents three bed reactor with two quenches. The maximum allowable bed outlet temperature is commonly +30°C compared to the inlet temperature (Alvarez, Ancheyta and Muñoz, 2007). Besides the cooling effect, the gas quenches also have other positive effects. Gas flow between catalyst beds reduces the hydrogen sulphide and ammonia partial pressures and replenishes some of the hydrogen that is consumed in the reactor (Alvarez et. al., 2007).

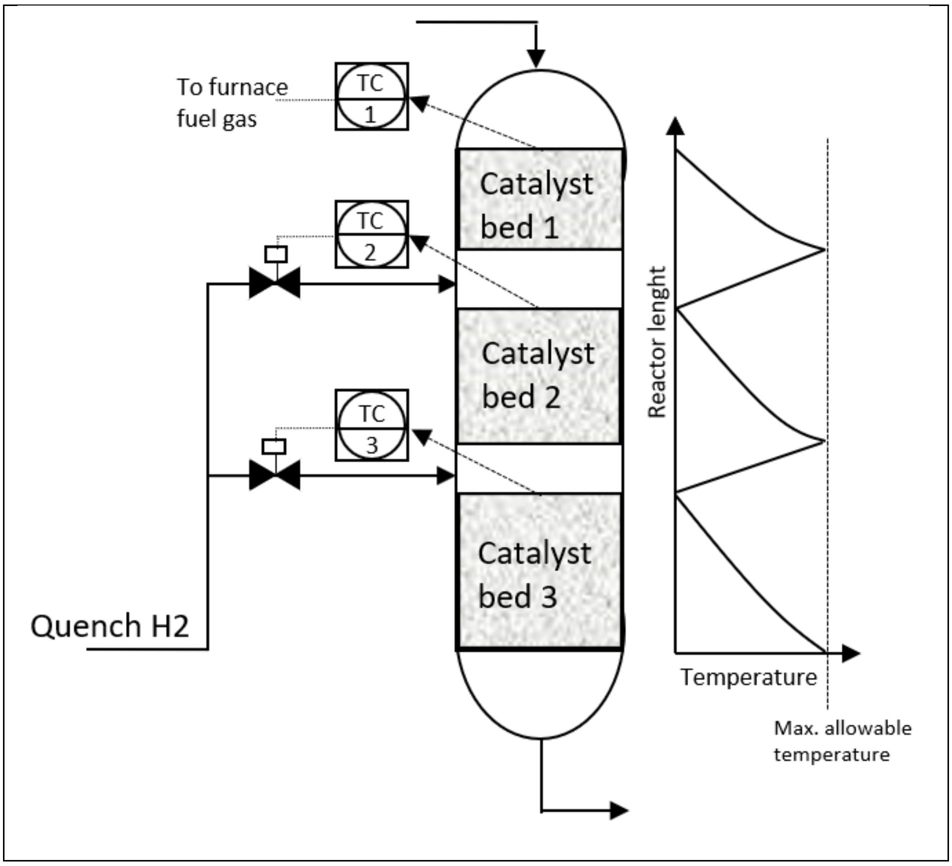


Figure 21 Three-bed reactor with two quenches (Alvarez et. al., 2007, modified)

Example temperature control setup, primary layer DCS temperature controllers and bed ΔTs are shown in Figure 21. Cooling between the beds keeps the temperature rice below max allowable maximum temperature. Panel operator gives setpoints for TC1-3, which adjust the furnace fuel gas and quench gas flows to control the inlet temperature of catalyst beds.

6 DCS-systems

Distributed control systems (DCS) are widely used to control large-scale production plants. Modern DCS systems have all the control and alarm functions that a panel operator needs when supervising and controlling production in a process unit. Distributed means, in this case, that the control systems are distributed on separate computers and servers which are connected through a process control network. The control system is distributed also geographically, increasing the safety of the system in abnormal situations. Large-scale continuous production plants in the chemical industry can have up to several thousand control loops and measurements to be controlled and monitored (Reddy and Mehta, 2015).

6.1 System hierarchy

The software hierarchy of a control system based on the ISO/IEC 62264 (ISA 95) is shown in Figure 22. Level 0 is the process, and the next level is the field instrumentation layer, which includes measurements and control valves. Above the field instrumentation layer is the process automation system (PAS). Older DCS systems did not have enough powerful historian properties, so third-party historians were used in level 3. Level 4 allows the communication from the DCS system to the office network (Berge, 2012; Reddy and Mehta, 2015; King, 2016). As the ISA 95 model shows the basic hierarchy layout, there are variations from this. In the refinery, where this thesis is made, there is a process information system which is located on level 3 but also partly on level 2. This system is briefly described in chapter 9.3.2.

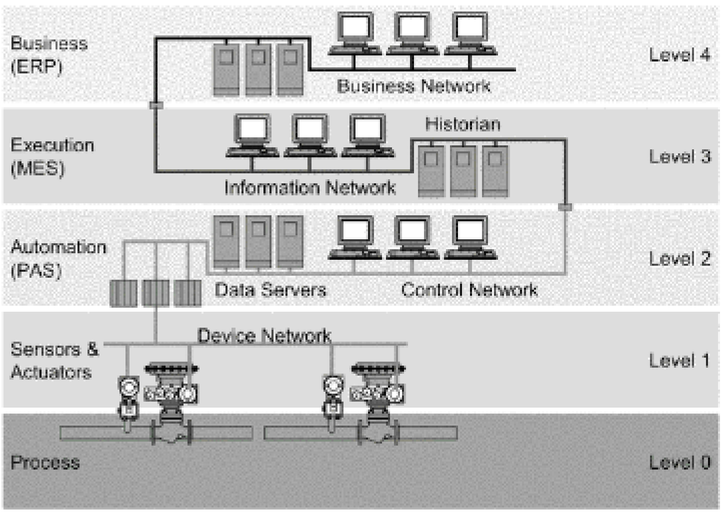


Figure 22 Software hierarchy in the ISA 95 model (Berge, 2012)

The APC controller will be located on level 3, and it communicates down to level 2 automation system setting setpoints for controllers that control the process.

6.2 PID-controller

PID-controllers are primary layer controllers using PID (proportional, integral, derivative) algorithms. They include basic temperature, flow and pressure controllers, which keep the process at desired conditions. Even they are base layer regulatory controllers, it does not necessarily mean that they are simple. They can have advanced techniques like feed-forward options, overrides and dynamic compensations. Regulatory means that the purpose of the controllers is to maintain the process conditions like temperatures, flows and pressures at desired set points (SP).

PID controllers have been in use since the 1930s, and they are the fundamentals of all basic-level controllers (King, 2016).

6.2.1 Feedback principle

PID controllers use the feedback principle (Åström and Hägglund, 1995). The main idea of how the controller works is that the controller is given a setpoint (SP). The measured process value (PV) is compared to the setpoint, and the deviation is the error (E). This is calculated with Equation 4 (King, 2016.). The size of the error and the rate of change define the controller actions, which is the output (u) going to the field device, e.g., the flow controller. For example, if flow controller setpoint is 50 t/h and measured value is 48 t/h, there is 2 t/h error. Controller output would increase, causing the flow controller valve to open more to minimise the error. As the deviation is measured, the controller is constantly doing corrective actions to minimize the error.

$$E = PV - SP \tag{4}$$

Where PV Measured process value

SP Controller setpoint

6.2.2 The modes of control

The proportional (P), integral (I) and derivative (D) terms affect how the controller output changes. Even though the controller type is PID-controller, it does not mean all terms are in use. P-term can be used alone in some cases, but PI is the most common combination. A controller with all modes of control in use, PID, is also used sometimes, but it is not very common (Wade and Harold, 2017). In general, if the PI combination gives enough good control, adding the D term is unnecessary, as tuning will be more complicated.

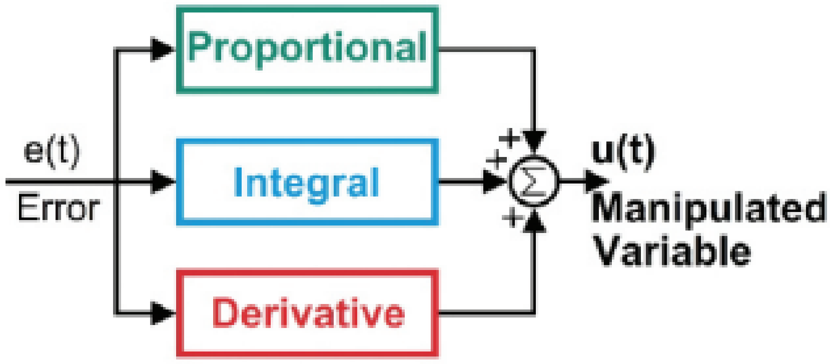


Figure 23 PID-controller (Rooholahi and Reddy, 2015)

The effect of each parameter is summed to the output value, as shown in Figure 23.

6.2.3 Proportion (P)

Proportional control is only proportional to the measured error between setpoint and measurement. High gain will cause the controller output to be increased if the error becomes high and vice versa. Too high gain makes the control unstable, and output can start to oscillate. P-control leaves a small control error, which can be corrected by selecting the correct bias. Equation 5 presents the proportional term and effect to controller output (Åström and Hägglund, 1995). For example, level control can be built using only proportional control.

$$u(t) = Ke(t) + u_b \quad (5)$$

Where	*u(t)*	controller output
	K	proportional gain
	E	error
	Ub	bias or reset

6.2.4 Integral (I)

Adding the integral action, the error that was present with only P-control, will be controlled to zero. Even if the error is small, it will lead to increasing control error, until the error is zero. In steady state situation with constant error the PI control signal is given by equation 6. (Åström and Hägglund, 1995)

$$U_0 = K\left(e_0 + \frac{e_0}{T_i}t\right) \quad (6)$$

Where	U_0	Control signal
	E_0	Error
	T_i	Integral time

Increasing integral time makes the controller more conservative, and short integral time makes the controller more aggressive.

6.2.5 Derivative (D)

Derivative action increases the closed-loop stability, and it is proportional to the time derivative of control error. It can predict future error as it measures the control error rate of change. Equation 7 shows the derivative term effect to controller output (Åström and Hägglund, 1995). Small changes cause small and large more significant changes to controller output.

$$u(t) = \left(Td\frac{de(t)}{dt}\right) \tag{7}$$

Where Td Derivative time

7 APC-controllers

Advanced Process Controllers (APC) are a significant concept, including many different control methods that are in additionally to basic control loops. Different cascades, overrides, ratio controllers and anti-windup functions also belong under the APC umbrella, but in the chemical industry, APC and Model Predictive Controller (MPC) are basically synonyms (Rhinehart, Darby and Wade, 2011).

7.1 MPC-controller

MPC controllers have a long history in process history. Richalet et. al. introduced 1978 model algorithmic control (MAC) by IDCOM (IDentificationCOMmand) (Corriou, 2018), but there was already in the 1960s linear growth in the number of process control computer applications (Bauer and Craig, 2008). Bauer and Craig (2008) surveyed over 60 industrial

APC experts, showing that the MPC-controller is the most common APC method nowadays. The use areas are diverse, from petrochemicals to the food and beverage industry.

MPC has a control algorithm, which uses process models to predict the future responses of the controlled process unit, and, using optimisation functions, control the unit efficiently against constraints (Darby and Nikolaou, 2012).

MPC controllers are efficient in continuous processes where the complexity is high and improved controllability increases profitability. Multiple input multiple output (MIMO) processes with long process dynamics, process constraints, and many manipulated variables (MVs) are good candidates for MPC control (Rhinehart et. al., 2011).

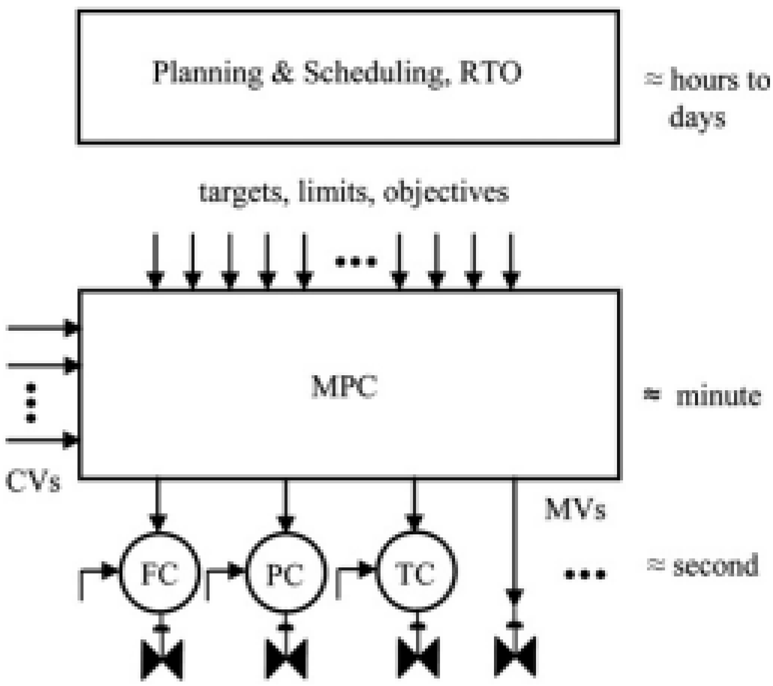


Figure 24 Plant control hierarchy (Darby and Nikolaou, 2012)

MPC controllers are positioned above the regulatory base layer controllers, as shown in Figure 24. The base layer controllers have a ~second execution rate compared to the MPC, which usually operates on 30 seconds to 1 min intervals. Over the MPC layer is possible Real-time optimization (RTO), which can give target setpoints to the MPC controller, but this layer is not necessary (Darby and Nikolaou, 2012). This thesis presents the main functions and structure of a linear MPC controller.

7.1.1 MPC control predictions and control horizon

The MPC controller uses process models to compute controller output over a future time horizon (Corriou, 2018).

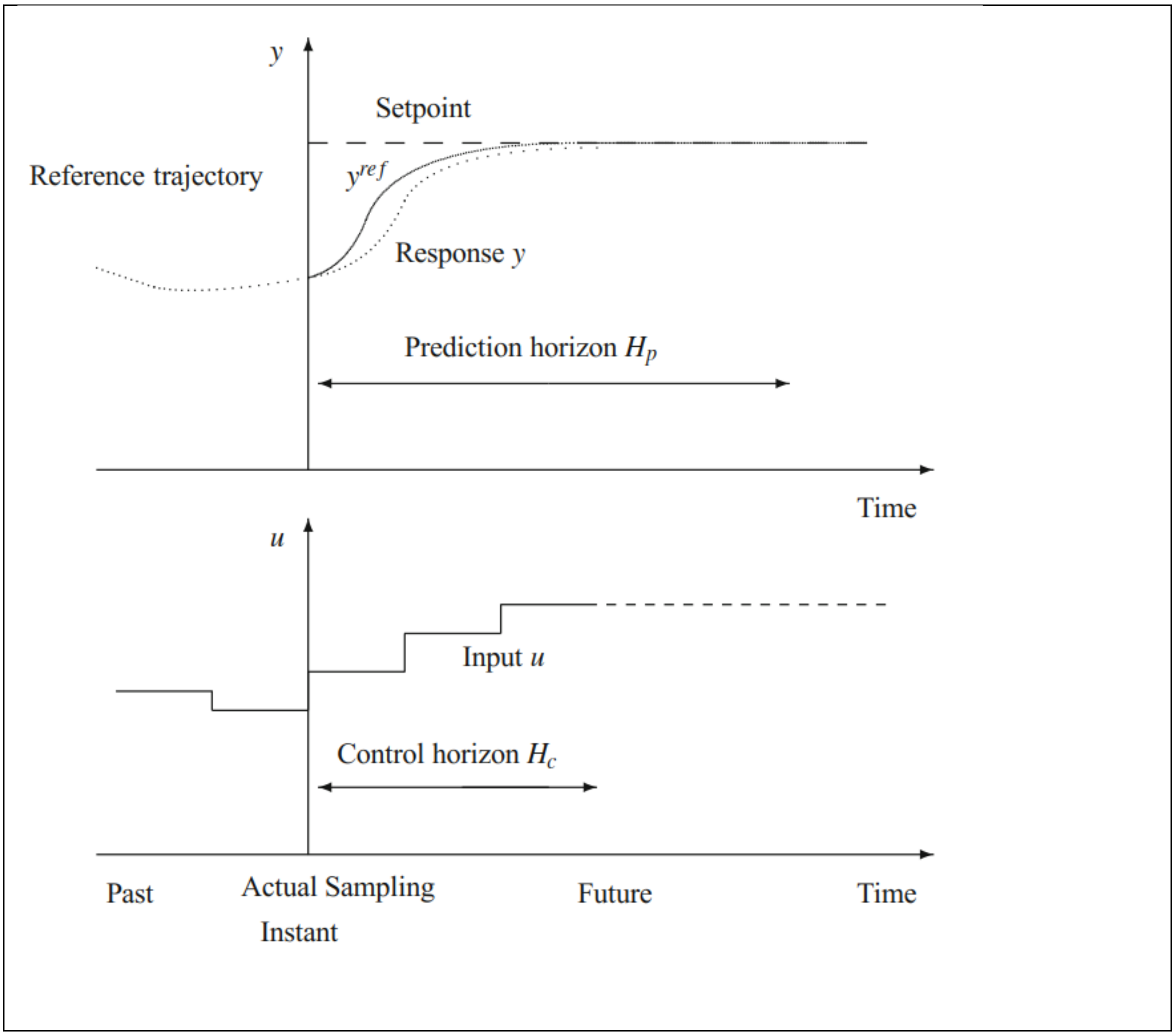


Figure 25 Principle of model predictive control with prediction and control horizon (Corriou, 2018)

Figure 25 presents controller actions, a reference trajectory (dashed line) is defined for the given time duration and the move plan for the manipulated variable (u) is calculated so that the future output values are as close as possible to the reference trajectory (Corriou, 2018).

Only the first move is sent to the MV setpoint, and the new move plan is calculated in the next controller execution cycle.

Qin and Badgwell (2003) describe the general objectives of an MPC controller in decreasing importance order:

- Prevent input and output constraints violations.
- Drive CVs to optimal steady-state values (Dynamic output optimization).
- If after controlling constraints and CV targets there is left degrees of freedom to control, drive MVs to their optimal steady-state values (Dynamic input optimization).
- Prevent unnecessary movement of MVs.
- If measured process signals fail or some MV cannot be used because of faulty device, control the plant still as much as possible using the remaining MVs.

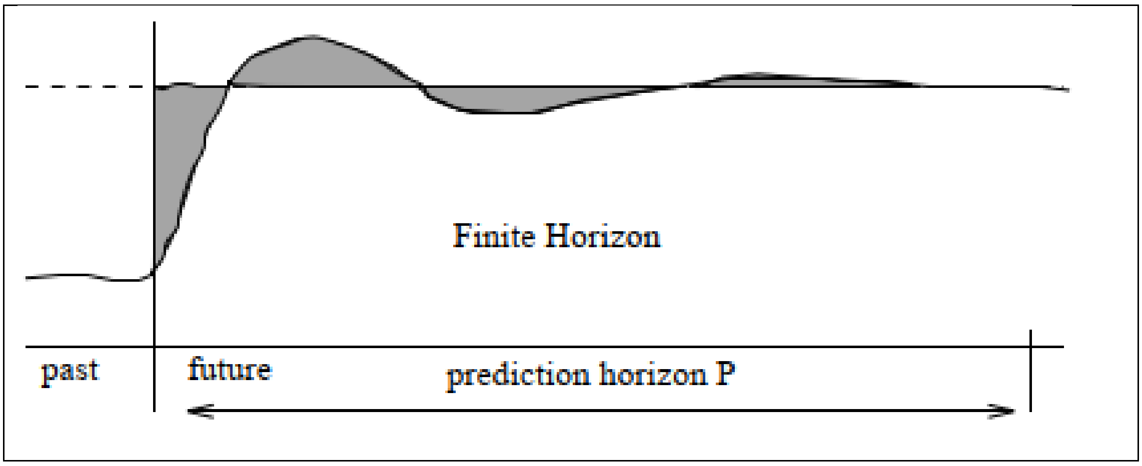


Figure 26 Output horizon (Qin and Badgwell, 2003)

In Figure 26, dynamic output optimization is driving CV on the upper limit. Shaded areas are penalised in the dynamic optimization.

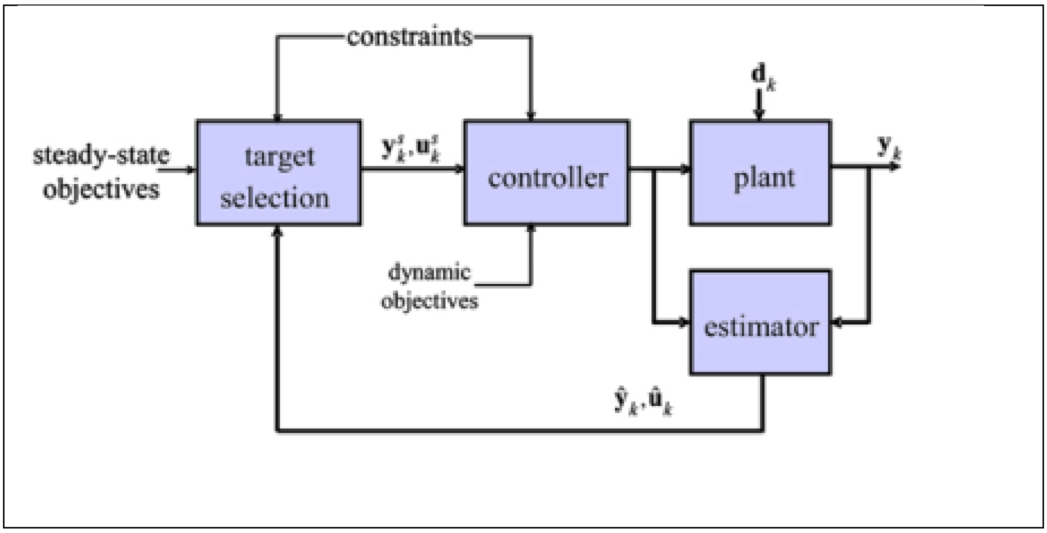


Figure 27 Figure 13 Simplified MPC block diagram (Darby and Nikolaou, 2012)

In the MPC block diagram (Figure 27), the target selection determines optimum steady-state values for CVs and MVs. The controller determines the move plan for the inputs how to reach the CV target and the estimator updates the model predictions. Bias between the measurement and model prediction is used to bias future model predictions (Darby and Nikolaou, 2012).

7.1.2 Commercial MPS products

There are many commercial vendors for MPC, and often the controller software is provided in a software package which contains tools for model identification and analysis and controller design and tuning tools (Rhinehart et.al., 2011). MPC applications usually operate on separate servers that are connected to DCS, but some DCS vendors have their own MPC products that are integrated directly into the control system (Logunov et al., 2020).

Qin and Badgwell (2003) did a survey in 2003 about MPC controllers usage in different industries. Twenty years ago, Aspentech DMC+, Adersa HIECON, Honeywell RMPCT, Shell Global Solutions SMOC and Invensys Connoisseur where few large companies and products mentioned then.

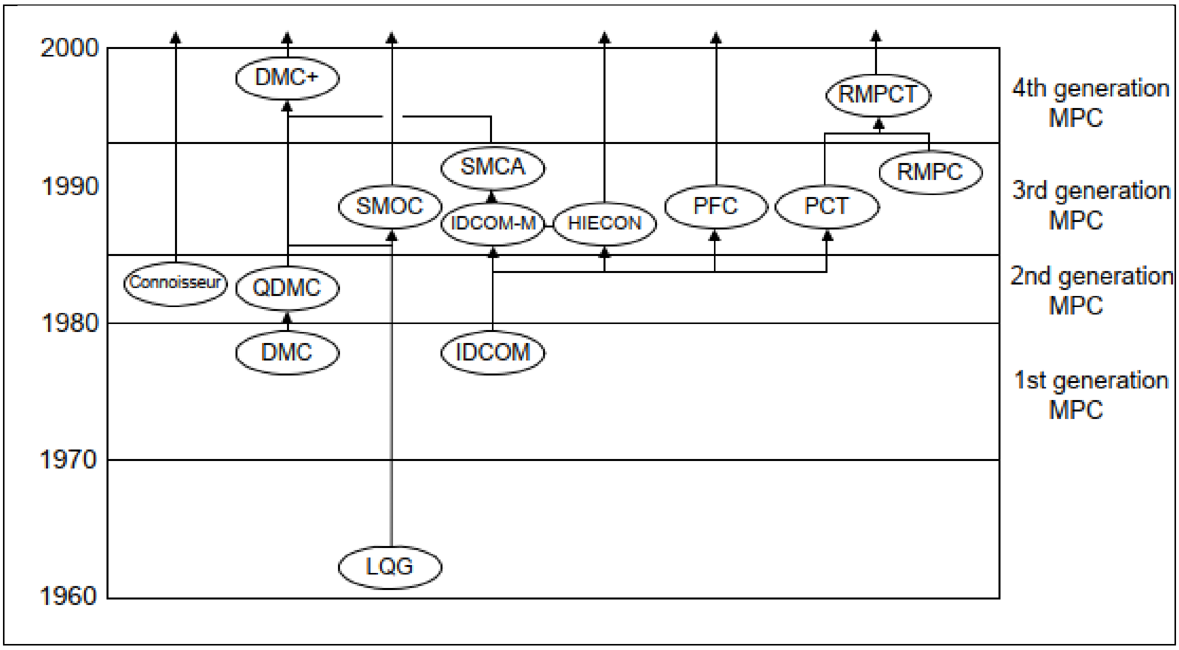


Figure 28 Approximate genealogy of linear MPC algorithms (Qin and Badgwell, 2003)

If a new study were done now, some company names would be changed because of mergers, and product names would be changed because of product updates.

Todays MPC basically uses the same algorithms that were developed during earlier generations of MPC. The focus of todays MPC is to improve the development steps, faster and easier controller commissioning, and the possibility of doing as much remotely as possible (simulatelive). Current controllers can also have features like MPC dashboards to measure and report performance using web-based technology (NAPCON).

7.1.1 MPC main variables

The simplified example distillation process in Figure 29 presents the main variables related to MPC control. MVs are marketed with red dots and CVs with yellow stars.

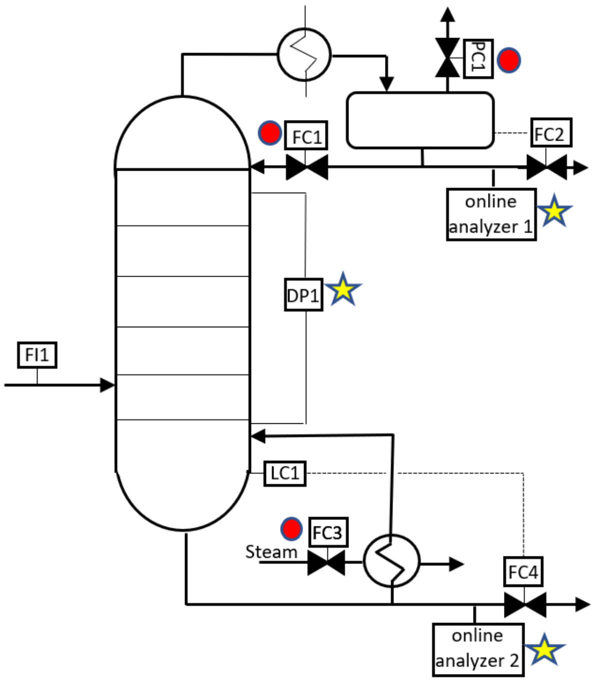


Figure 29 Simplified distillation column, controlled and manipulated variables

7.1.2 Manipulated Variables, MVs

MVs are normally PID controllers setpoints that are executed in the DCS. MVs are often flow, temperature, or pressure controllers, which setpoints the operator can change from the DCS, and when using MPC, these setpoints come from the MPC controller. It is also possible to manipulate valve positions directly with MPC bypassing the PID-control loop (Darby and Nikolaou, 2012). MVs are independent variables that are not depending on other variables. MVs in the Figure 29 process are the bottom reboiler steam FC3, the top reflux FC1 and the reflux drum pressure controller PC1.

7.1.3 Controlled Variables, CVs

CVs are dependent variables, which change, e.g. because of the change in independent variable.

CVs are the measured or calculated process values the controller controls at the selected setpoint. CVs can be, e.g. reactor temperature, product quality from distillation column or measured excess oxygen from furnace flue gas.

CV targets can be exact setpoint target values, min/max values, or zone CVs where the target value has minimum and maximum values defining the allowed control zone. CV with the maximum value in Figure 29 process could be the column pressure difference DP1. A low pressure difference is not concerning, but if the DP1 is close or over the maximum limit, it can be a sign of column flooding, and the controller needs to do correcting actions with MVs. Other CVs are top and bottom product qualities, which are measured with online analysers.

7.1.4 Feed-Forward variables (FF)

Feed-forward variables (FF) are independent variables, like MVs. The change in the FF variable causes CV values to change. FF variables cannot be controlled or wanted to be controlled with the controller. The controller performance is better when the FF variables are also modelled, and the controller can do corrective movements with MVs when there is a change in the FF variable. The column feed flow measurement FI1 in Figure 29 could be a feed-forward variable.

7.1.5 Models and identification technology

Forecasting the process behaviour and optimising it with MVs are the main tasks of an MPC controller. Process models are the main elements that the MPC controller uses for these purposes.

Controller vendors use different model forms and types, typical are Finite impulse response (FIR), Finite step response (FSR), Laplace transfer function and linear state-space (LSS) models.

Finite impulse response (Equation 8) uses 30 to 120 coefficients to describe the full open loop response (Qin and Badgwell, 2003)

$$y_k = \sum_{i=1}^{N_u} H_i^u\, u_{k-i} + \sum_{i=1}^{N_v} H_i^v\, v_{k-i} + \sum_{i=1}^{N_u} H_i^w\, w_{k-i} + \xi_k \tag{8}$$

Where Y_k output

H_i impulse response coefficients

u_k MV vectors

v_k FF vectors

w_k state disturbance

ξ_k measurement error/noise

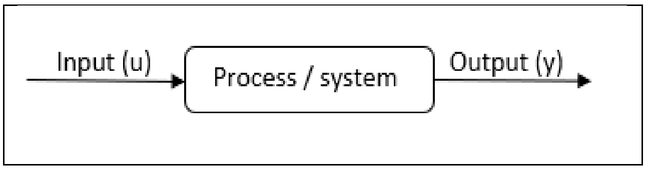


Figure 30 System input and output

Transfer functions are one method to present the process, the input and the related output (Figure 30). In control engineering, transfer functions are formed via Laplace transform (Kippo and Tikka, 2008). Laplace transforms converts time domain variable (t) into frequency domain variable (s) (Henttonen and Peltomäki, 2006). Some controller algorithms have the possibility to use a Laplace transformed function model, and the controller then automatically transfers it to a discrete time model that is used in the control calculations (Qin and Badgwell, 2003). Process transfer function G_p presented as the relation between Laplace transferred output and input (Equation 9).

$$G_p(s) = \frac{Y(s)}{U(s)} = \frac{Ke^{-T_e s}}{T_b s + 1} \tag{9}$$

Where	G_p	Process transfer function
	$Y(s)$	Laplace transformed output
	$U(s)$	Laplace transformed input
	T_b	Process time constant
	K	Process gain
	T_e	Process dead time (s)
	s	Laplace variable

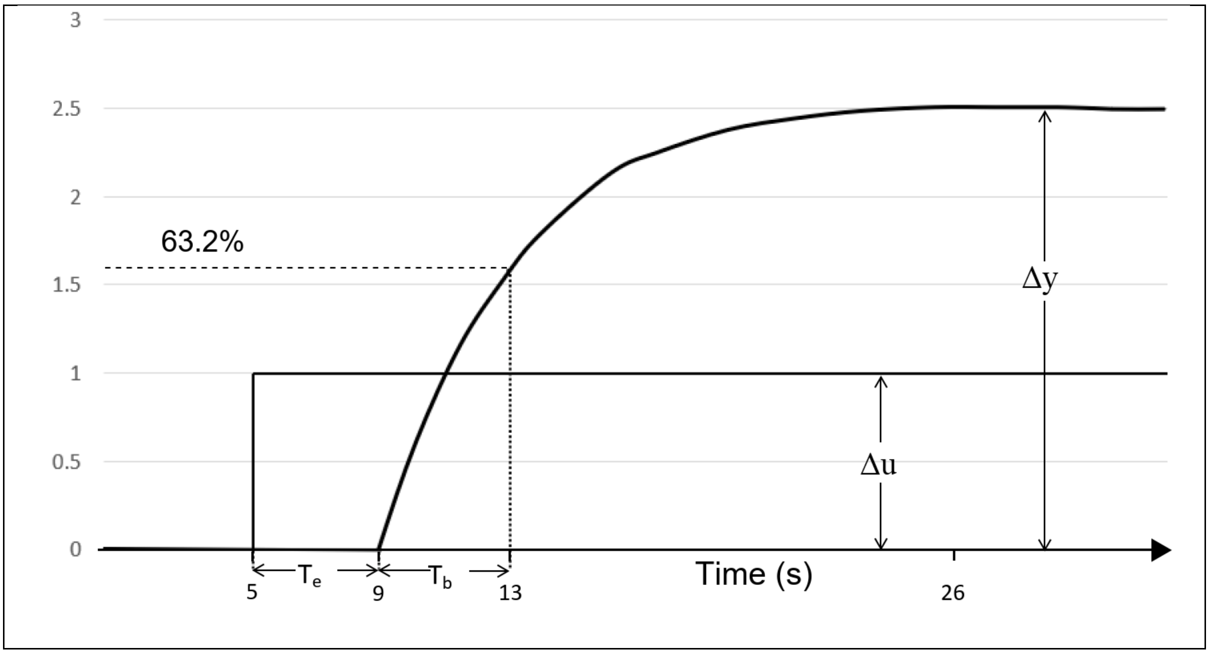


Figure 31 First order step response diagram (Kippo and Tikka, 2008 modified)

Process variables deadtime (Te), time constant (Tb) and gain (K) can be defined from a step response diagram (Figure 31). The process input variable is changed from 0->1 on time point 5 seconds. Output variable starts to change at time point 9 seconds, so the process delay, dead time is T_e =9s – 5s = 4s

The time constant is the time when the output variable has reached 63.2% from its final value compared to the beginning of the step response. The output variable started to increase at time point 9, and it reached 63.2% of the final value at time point 13, so the time constant is 13s – 9s = 4s.

Process gain is the Δy / Δu, so gain K is 2.5.

7.1.6 MPC controller advantages

MPC controllers are often beneficial tools to improve, e.g. process unit performance, and project pay-back time can be very short. Bauer and Craig (2008) report that the bay-pack time of an APC project is generally 3-9 months. Besides economic benefits gained from improved process controllability, it can also ease the panel operator workload by controlling and optimizing specific parts of the process unit, allowing the operator to do other more profitable operations in the remaining part of the process unit.

As King (2011) and Logunov et al. (2020) point out, the MPC controllers facilitate operators work, but they cannot replace operators, and the aim of an MPC project is not to reduce the workforce. Controllers are good tools, but they need human follow-up, operations and intervention if needed.

Rhinehart et. al., (2011) point out also adverse effects, that MPC controllers can cause for operators. At least regarding new operators, they can reduce process understanding when manual operations are more seldom. This should be taken into consideration regarding operator training. Todays efficient solution for the training of plant operators is e.g. accurate training simulators that can be used to train process upsets and normal operations (NAPCON).

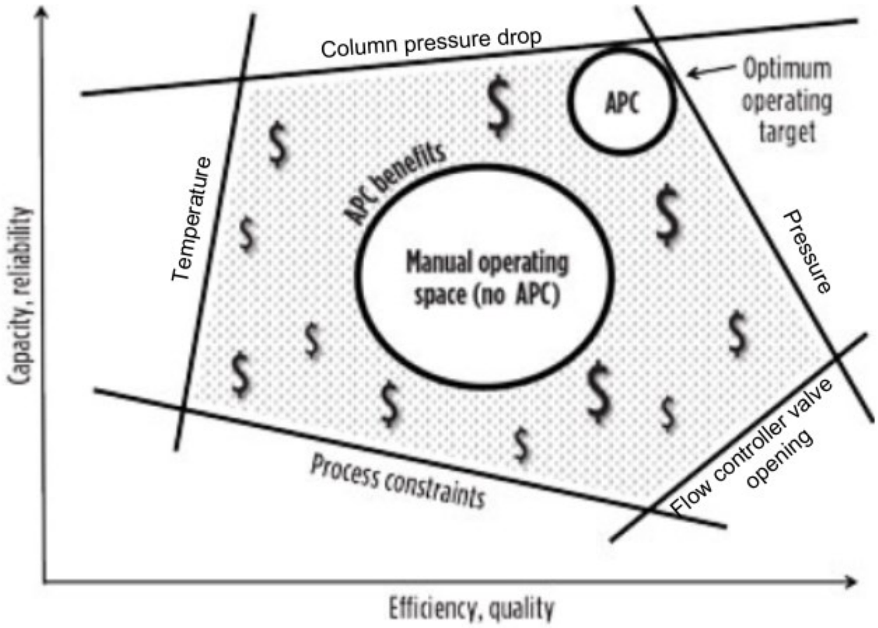


Figure 32 Manual unit operation vs. APC (Kern, (2018), modified)

The basic idea, of how APC-controller can increase the unit profitability, can be seen in Figure 32. The process is always constrained by some constraints that cannot be exceeded. High distillation column pressure drop can be a signal of an overloaded and flooding column, pressure can be limited based on the maximum pressure of safety relief valves, and temperature can be limited based on material limitations, to mention a few possible constraints. Process operation is the most beneficial when the process is against actual process constraints, as shown in Figure 32.

Operating the process using DCS-layer controllers, the operator needs to keep the process in the safe middle zone, with enough safety margin against process constraints. This can result, for example, lower yield and energy efficiency. (Kern, 2018)

When asked by over 60 APC experts (Bauer and Craig, 2008) about their main MPC controller profit contributors, the TOP 5 list was:

- Throughput increase

Canney (2003) estimated that process unit feed could be increased by 3-5 %, with no change in product quality using an MPC controller. This is beneficial if the increased feed leads to increased products, which can be sold at the same unit price.

- Process stability increase

If the process is more stable, it also leads to more constant and steadier product quality.

- Energy consumption reduction

Energy consumption reductions depend on the process and controller design. MPC controller does not automatically reduce energy consumption, but it can be a powerful tool to optimize energy usage if needed.

- Increased yield of more valuable products

It is possible to increase the amount of more valuable products with better controllability. E.g. in distillation separation, distillates commonly have different values, and MPC controller can maximize the most valuable product or products.

- Quality giveaway reductions

Quality giveaways can cause significant monetary losses in some cases. Product quality, which is too “good” compared to the product spec, can increase energy consumption, but the product price remains the same.

7.1.7 Process constraints

Process constraints can be divided into soft and hard constraints (Figure 33). Hard constraints should be approached only from one side, e.g., maximizing pressure against pressure relief valve (King, 2011).

Soft constraints can be violated for a short time, e.g. product quality can be violated for a short time if the product goes to a large storage tank (King, 2011).

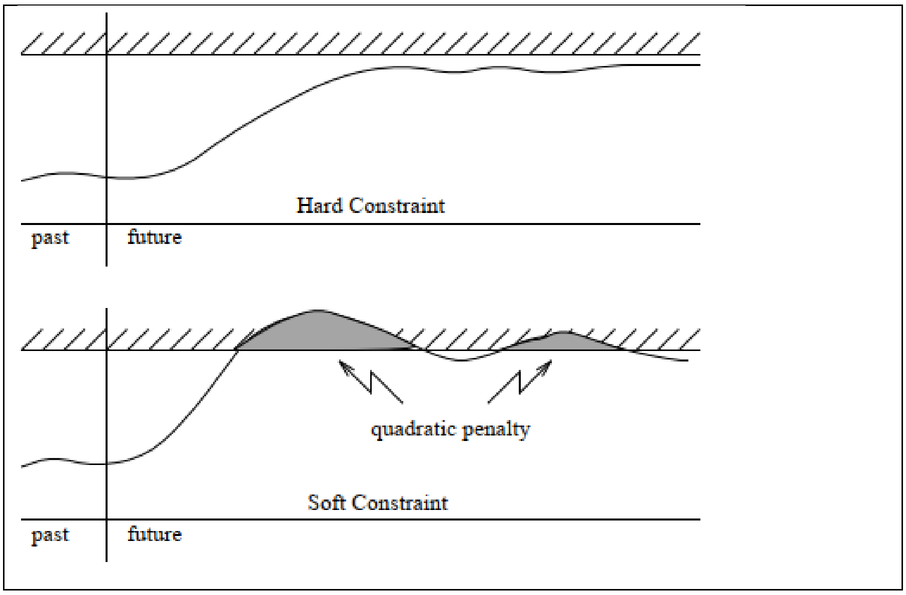


Figure 33 Hard and soft constraints (King, 2011)

A most common method of the MPC controllers is to use the quadratic objective function for dynamic optimization (Equation 10) (Qin and Badgwell, 2003).

Dynamic objective function is minimized to compute MV setpoints, which would drive the process to the desired steady-state operating point with (Kazancoglu, Ozbiltekin-Pala and Ozkan-Ozen, 2021)

$$J(u^M) = \sum_{j=1}^{P} \left\{ \left\| y_{k+j} - y_{k+j}^r \right\|_{Q_j}^2 + \left\| s_j \right\|_T^2 \right\} + \sum_{j=0}^{M-1} \left\{ \left\| u_{k+j} - u_s \right\|_{R_j}^2 + \left\| \Delta u_{k+j} \right\|_S^2 \right\} \quad (10)$$

Where $y_{k+j} - y_{k+j}^r$ is the deviation from the desired output trajectory, it is minimized over prediction horizon length P.

Sj, output constraint slack variable, size is minimized over prediction horizon length P

$u_{k+j} - u_s$ is the deviation from the desired steady state inputs, it is minimized over control horizon length M.

Δu_{k+j} term is used to minimize rapid input changes

8 MPC-controller implementation project

8.1 Project steps

Several separated process phases can be defined when building a new MPC controller. The first task is to do a study related to the process unit and estimate the possible benefits that could be attained with the improved controller. The project to commission the controller can be divided into different project steps, Darby and Nikolaou (2012) have divided the project as follows:

- Pretesting and preliminary design phase
- Plant testing, often step testing
- Modelling and development of the controller
- Commissioning if the controller and user training

8.1.1 Benefit estimation

A benefit estimation document is one of the first documents that is produced. The process where the controller is planned to be implemented is carefully studied, and an estimation regarding the costs and benefits is done. Bauer and Craig (2007) study results showed, that 60% of cost benefit analysis regarding MPC was done by the users, and 40% by the suppliers. The size of the organisation and knowledge related to optimization and MPC opportunities are affecting the possibilities for the users to produce cost estimation documents by themselves. The cost/benefit estimation is one main factor that affects the decision of whether the MPC controller will be implemented or not. King (2011) points out, that benefits should be related to actual process performance and should be calculated with reasonable accuracy. Overestimating the benefits can ease the approval process for the project, but if they are not achieved, the approval project for the next controller will be more challenging. On the other hand, being too conservative and underestimating benefit calculation results may stop promising controller ideas from being implemented.

As the improved controllability can increase process stability, the process can be operated closer to hard constraints limits, e.g. product quality limit. Figure 34 shows improved control and reduced standard deviation.

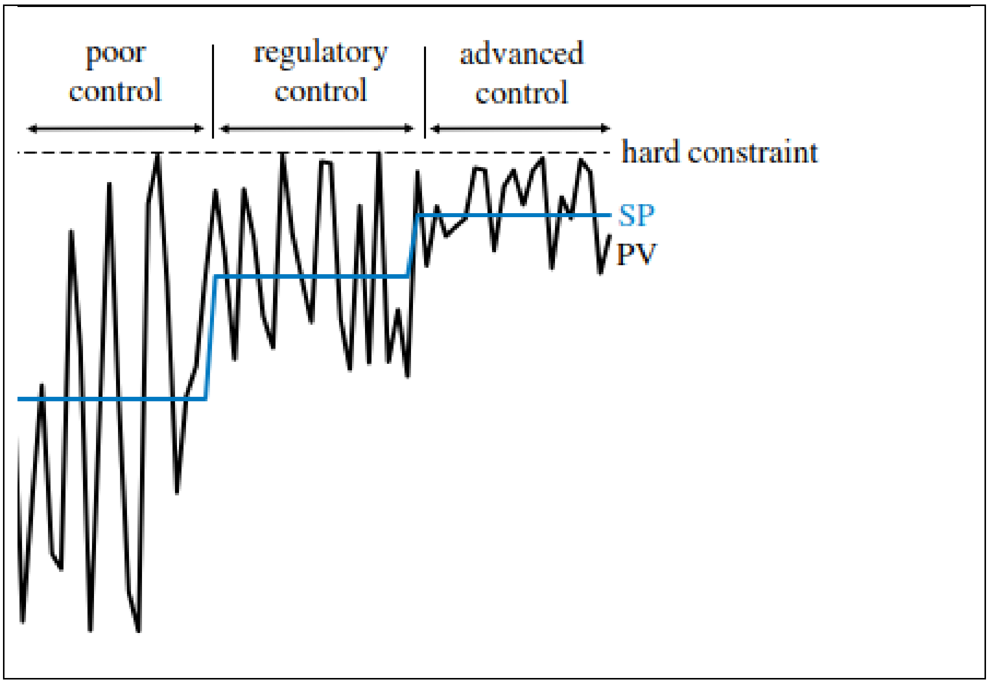


Figure 34 Improved control benefit versus hard constraint (King, 2011)

King (2011) presents an industrial rule of thumb that improved regulatory level control using e.g. MPC halves the standard deviation. There is no theoretical background in this assumption; it is based on post-implementation studies. The estimated reduced standard deviation can be used in benefit estimations using the same percentage and same limit rules.

8.1.2 Same percentage rule

If it can be assumed that some percentage of results violate the hard limit before improved control, it can be allowed that the same percentage of results can violate the limit also after control improvement (King, 2011). Figure 35 presents collected data, where the process unit product is normalized to a percentage of specification, and the y-axis is the cumulative frequency of the samples. Operating close to the maximum limit would be economically feasible in this example. Black lines present the best fit normal distribution; the blue line is the distribution if the improved control improves the standard deviation by 50%.

Before the improved control, the average of the results was 97.5%, and the standard deviation was 2.3%.

As the improved control halves the standard deviation, also the average deviation from the target can be halved:

$$\Delta\bar{x} = 0.5 * \left(x_{target} - \bar{x}\right) = 0.5 * (100 - 97.5) = 1.25 \tag{11}$$

Where	x_{target}	is the specification limit 100%
	$\bar{x}$	is the average of the samples

As a result of improved control, the process can be operated closer to the maximum limit, and the mean result increases from 97.5 to 98.75 (Equation 11). The same number of results will violate maximum limit after the improved control giving the same percentage of violation of maximum limit.

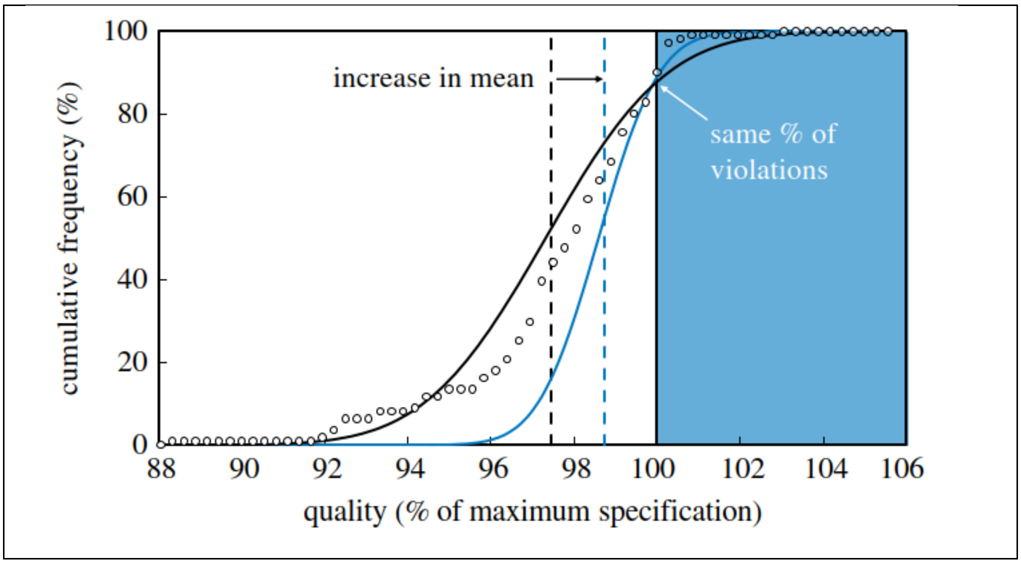


Figure 35 Same percentage rule (King, 2011)

How to change the better controllability and possibility to operate closer, e.g. specification limits to monetary value, depends on the production process and from case to case.

An increase in main product streams, which have strict quality specification limits, energy consumption reductions, or an increase in whole production unit feed can often easily be converted as monetary value.

Quality or mass change in streams, which are from one process unit to another process unit, can be more difficult, as the intermediate value is not easy to define, or they can change from time to time. Price estimates from the refinery production planning department or LP model as Logunov *et al.* (2020) have used gives enough accurate prices for the intermediate products. The LP model is a linear programming mathematical model that models the whole refinery and is usually used, e.g., as a production planning tool.

E.g. in the petroleum industry, MPC controllers are often used to optimise distillation column operations like distillate qualities, cut points between different components from multicomponent distillation towers etc. If one side withdrawal amount is increased, that causes the opposite change in some of the other column product flows, the other qualities will also change. Changed quality properties may decrease the value of other streams, which must be also considered in the total calculation process. Knowledge and understanding of material balances and unit processes are needed to design the controller and estimate the benefits.

Increased energy efficiency that would decrease CO_2 emissions can also benefit economically as carbon pricing sets high prices for emissions now and higher costs in the future. In the European Union Emission Trading System (EU-ETS), carbon dioxide emission price varied between ~60 to 100 €/t from January 2022 to September 2023 (Statista.com), and it is estimated that the price may achieve ~150 €/t in 2030 (GMK Center).

8.1.3 Pretest and preliminary design phase

A preliminary design phase is needed in the beginning, e.g. to select the controlled and manipulated variables (Darby and Nikolaou, 2012). When all manipulated variables are known, the pretest phases and possible PID-controller tuning can be started.

Pretesting is done mainly to check the DCS controllers performance and that the instrumentation, like temperature, flow and pressure measurements, are sufficient and working. Pretesting is done by changing the setpoints of planned manipulated variables, and it reveals if the controllers can control the process enough fast and accurately. MPC-controller is over base layer DCS controllers on the hierarchy level. Most common structure is to give set points from MPC-controller to DCS controller and DCS controller need to be able to respond fast and accurately to setpoint changes. A sluggish and slow DCS controller decreases the controller performance. Also, poorly working controller valves, mainly because of valve stiction common problem (Rhinehart et al., 2011). Sticky valve behaviour causes rough control performance, and it can be caused, e.g., by the wearing of valve inner parts.

8.2 DCS tuning

The hierarchal structure requires that the regulating level controllers and instrumentation are working at a satisfactory level. The pretesting phase can reveal a control loop that requires tuning. DCS control loop tuning mainly defines and seeks the PID tuning parameters that would result to desired controller performance. One part of MPC-project benefits can come from the PID-controller tuning work performed during the project (Darby and Nikolaou, 2012).

The tuning parameters can be determined using classical methods, like the Ziegler-Nichols step response method or the Frequency Response method. Tuning methods can give at least reasonable starting point tuning parameter estimates, which can then be continued based on the process response. Often, different tuning methods can give first estimated parameters, but process and control knowledge are needed to estimate the sensibility of parameters.

Tuning performance criteria depend on the process and controlled substance. Figure 36 presents setpoint response and performance-related metrics. Rise time (T_r) is how fast the controlled variable reaches the setpoint. If the setpoint is changed often, minimization of rise time can be important, e.g. MPC-controller manipulated variables setpoints are often changed. Fast control (Figure 36) can cause overshoot E_{x1} and undershoot E_{x2} as more sluggish control reaches the setpoint slower, but there is no overshoot. Too significant overshoot can cause process runaway in temperature-sensitive processes or trigger a safety instrumented system (SIS). Temperature undershoot on the other hand can reduce conversion, e.g., reactors (McMillan, 2015. pp110).

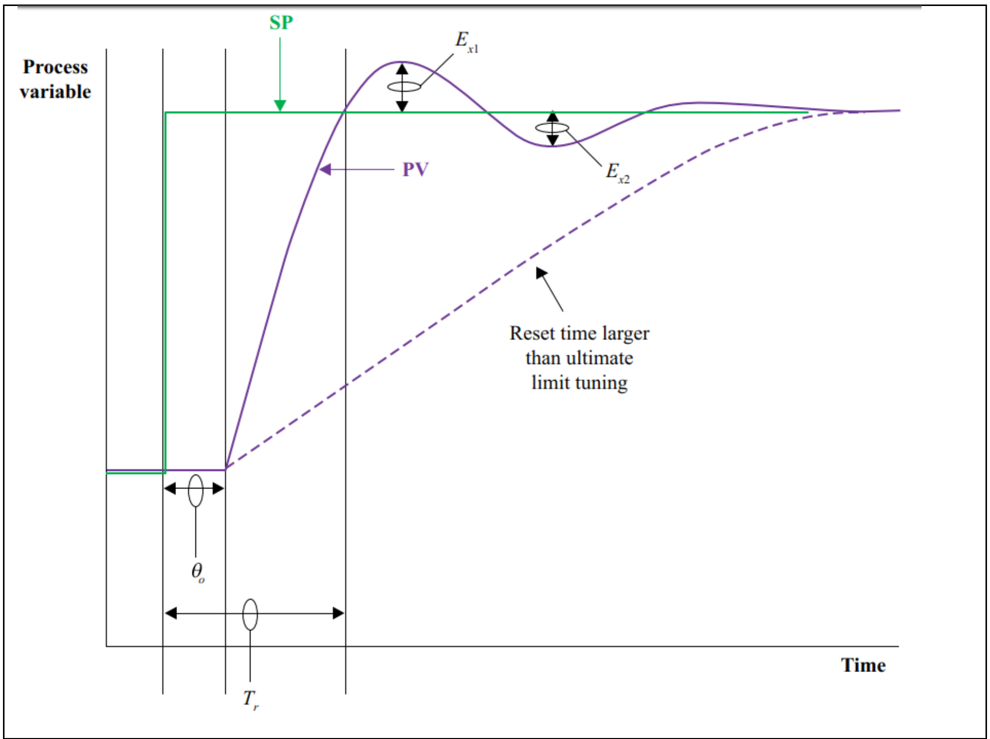


Figure 36 Rise time (Tr), overshoot (Ex1) and undershoot (Ex2) (McMillan, 2015)

Table 4 presents the effect of individual changes of P, I and D terms in steady-state situation. These can be used as a rule of thumb, but the parameters are also related to each other, so one may not be independently changed. McMillan (2015) warns, e.g. not to reduce integration time too much if the maximum gain is not used.

Table 4 Changing individual Kp, Ki or Kd parameters and the steady state effect. (Rooholahi and Reddy, 2015)

Parameter	Rise Time	Overshoot	Settling Time	Steady-State Error	Stability
Increasing K_P	Decrease	Increase	Small Increase	Decrease	Degrade
Increasing K_I	Small Decrease	Increase	Increase	Large Decrease	Degrade
Increasing K_D	Small Decrease	Decrease	Decrease	Minor Change	Improve

Manually testing the effect of changing tuning parameters is a working tuning method, but it can be time-consuming. Many trial and error steps can be needed to reach the final parameters, and there is always a need to follow the process after the changes for some time to ensure that the changes are not causing instability in different operating values and zones.

8.2.1 Ziegler-Nichols step response method

Ziegler-Nichols method is done using step response from an open loop step change and defining two parameters, α and L, from this result (Åström and Hägglund, 1995). These two parameters can be used to determine PID parameters using related tables.

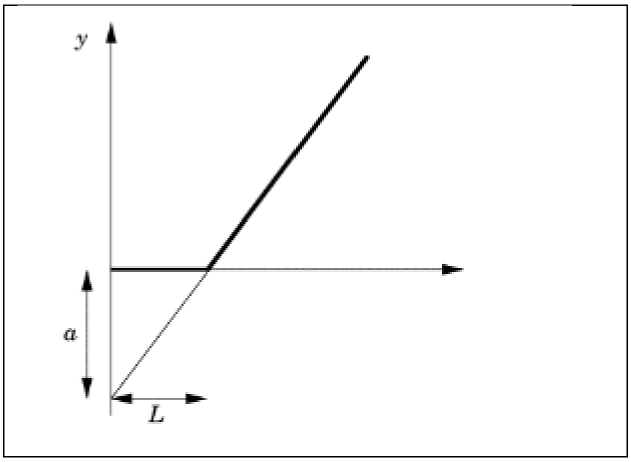


Figure 37 Step response in the Ziegler-Nichols step response method (Åström and Hägglund, 1995)

In the step response method, the step test for the controller is done in open loop mode, meaning that the controller is not in the normal automatic mode, and no setpoint–measurement error feedback is used. Stepwise change is done for the controller output, e.g. control valve position, and the response is drawn in an x-y plot.

Figure 37 shows the step response and α and L parameters. The tangent is drawn from the point where, the slope of the response is at maximum. From the x-axis intersection can parameters α and L be determined, and tuning parameters are shown in Table 5.

Table 5 Table to define tuning parameters (Åström and Hägglund, 1995)

Controller	K	Ti	Td
P	1/α		
PI	0.95/α	3L	
PID	1.2/α	2L	L/2

8.2.1 Ziegler-Nichols frequency method

The frequency method is another traditional tuning method. The idea is to find the parameters of ultimate gain (K_u) and ultimate period (T_u). A practical method to obtain these is to have the controller in closed-loop mode. Integration time is set to infinity, and the derivation parameter is set to 0, so only the proportional K parameter affects the control. The gain (K) parameter is gradually increased until the controller starts to oscillate. This gain is the K_u, and the oscillation frequency is the T_u parameter, and the PID-controller parameters can be read from Table 6 (Åström and Hägglund, 1999).

Table 6 PID controller parameters from frequency method (Åström and Hägglund, 1995)

Controller	K	Ti	Td
P	0.5 K_u		
PI	0.4 K_u	0.8 T_u	
PID	0.6 K_u	0.5 T_u	0.125 T_u

Åström and Hägglund (1995) point out that these Ziegler-Nichols methods only estimate the tuning parameters and manual tuning is also needed to achieve the desired performance. The step response method generally gives higher gain values than the frequency method. Comparing these methods, with the frequency method it is more straightforward to determine the parameters K_u and T_u from the process test data. Still driving the control loop on oscillation state is not possible in all cases, like in sensitive reactor temperatures.

8.2.2 Plant testing and modelling

Plant testing, mainly step testing, is an important phase to generate plant data for model identification. It includes moving all independent variables that are considered as possible controller MVs. The step-testing phase is also essential, as it can generate helpful process knowledge (Darby and Nikolaou, 2012).

Standard method for plant step testing is the traditional step testing, where stepwise change is done for one manipulated variable at the time, and data from the step test is collected. This data is used in the modelling phase for empirical model identification. Empirical models are derived from process test data compared to first-principle models that are based on theoretical foundations like mass and energy balances (Qin and Badgwell, 2003).

The plant testing phase is time-consuming, and it can take up to 50% of the project time (Darby and Nikolaou, 2012). The plant testing phase requires an APC engineer to follow and monitor the step testing in the control room, and if tests are done in day and night shifts, they require enough personnel in the project group.

Some new MPC-control products also offer the possibility to perform automated closed-step tests. Controlled needs an initial model to start with, which can be oriented, e.g. from manual step tests, and then it can perform small automated step tests to gain more data accuracy (Darby and Nikolaou, 2012). The traditional step testing phase usually is still needed, at least on a small scale, to identify the “seed model” where to start.

Step sizes are selected large enough that the response is visible enough. (Darby and Nikolaou, 2012) sets the goal for the response so that the signal-to-noise ratio should be 5-1, meaning that the response should be five times bigger compared to the normal noise that is presented in the measurement. Step sizes are usually agreed with the unit panel operator and plant engineer so, that they are large enough to provide the needed feedback, but not too big to cause process upsets, pushing the process out from the safe operations window, that is limited by hard process or product quality limitations.

The modelling part starts when enough plant test data is collected. Modelling is usually done using the model identification package that is provided with the controller software.

After successful modelling part can control system related configuration work continue to build the actual controller. Controller functionalities can be tested using possible controller simulation options before actual commissioning phase to ensure the desired controller behaviour.

8.3 Controller commissioning and training

Before the controller commissioning, the possible change in process unit operations needs to be examined from different angles, and the process safety is one of the most important. If the MPC controller operates the unit in the same operating window as when operating without the controller, there should not be changes in that. Operating window is limited by certain hard limits, like temperature, pressure or flow or other process parameter limits, and those hard limits are configured into the controller with some safety margin. But it also possible that during process testing some new operating modes or limits are found, and the controller will be operating the process differently compared to previous. All changes and the possible effects should be studied in a systematic method, e.g. using suitable Management of Change (MOC) tool. King (2016) recommends the use of the Control, Hazards and Operability (CHAZOP) or Failure Mode Event Analysis (FMEA) tools at least if there is a major process revamp.

Panel operator training is an important phase of the controller commissioning. Operators need to understand the controller structure, objectives and how to operate it. If the operators do not have confidence in the controller or they do not understand how and why it controls in the way it does, the controller will easily be turned off. A common problem is which also (Darby and Nikolaou, 2012) point out is the MV limit pinching. Operators can start to pinch MV limits to keep it in the area that they are used to operate, and it causes decreasing MPC performance, causing losses in the controller benefits. Controller cannot use MVs optimally, and it can also result in unwanted controller actions. Engineer support and hands-on training for the operators in the control room during the implementation is a good method to increase the controller knowledge.

8.4 Successful MPC-project

MPC projects can have varying success rates. The selected MPC technology is not the key to a successful project; it is more a combination of skilled personnel and sufficient resources in the project group. Also, management commitment to the deployment and support for the project is essential as (Darby and Nikolaou, 2012) point out.

King, (2011) presents a Kepner-Trago analysis results (Table 7) that can be used e.g. in MPC-vendor selection process, but it also clarifies some important factors related to potential benefits.

Table 7 Kepner-Trago analysis (King, 2011)

Key issues	Potential benefits	k$	Rating (%)	Value
Training of own personnel	50% cost saving in the next project	150	50	75
Selected inferential technology	Cost of analyzer + 9 months benefits	175	70	123
Experienced lead engineer	20% of total benefits for three years	600	85	510
Vendor support, quality and location	Three faults/year fixed one day earlier	25	100	25

Even though the analysis was done in 2011, the potential savings are still probably on the same scale nowadays. The most critical factor listed here is the lead engineer quality, as the lead engineer role is essential during the project. Controller design, e.g. regarding the controller structure, model matrix, and selecting the right CVs and MVs, are fundamental decisions that are done in the early project phase. The lead engineer has an important role during all the significant steps during the implementation project, and also, at least some part of the other project group members should be experienced in APC controller project implementation. A project that has an unexperienced project team has the low possibility of being able to design and implement a working MPC controller despite the tools that they are using.

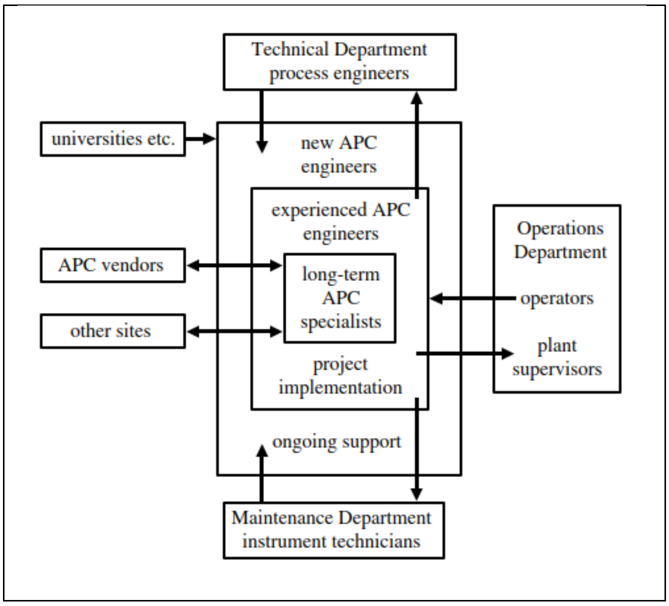


Figure 38 Example of APC-personnel rotation in organisation (King, 2011)

(King, 2011) shows one example of a working APC group in Figure 38 and how the personnel could be rotating in different organisations and positions. King mentions that in his experience, most successful APC-engineers are former process operators. Their strong knowledge of the process and how to control it must be the reason for this.

9 Experimental work

The experimental part of this thesis is the development and implementation of an APC-controller in a hydrotreating reactor in a petroleum refinery. The future plans to begin biobased feed co-processing in this reactor were the driver to enhance the current reactor temperature controlling system. Currently, the panel operator manually sets setpoints for the DCS controllers, which can be time-consuming and not a very accurate method to control reactor temperature. Also operating close to process constraints is not possible effectively.

9.1 Hydrotreating reactor process

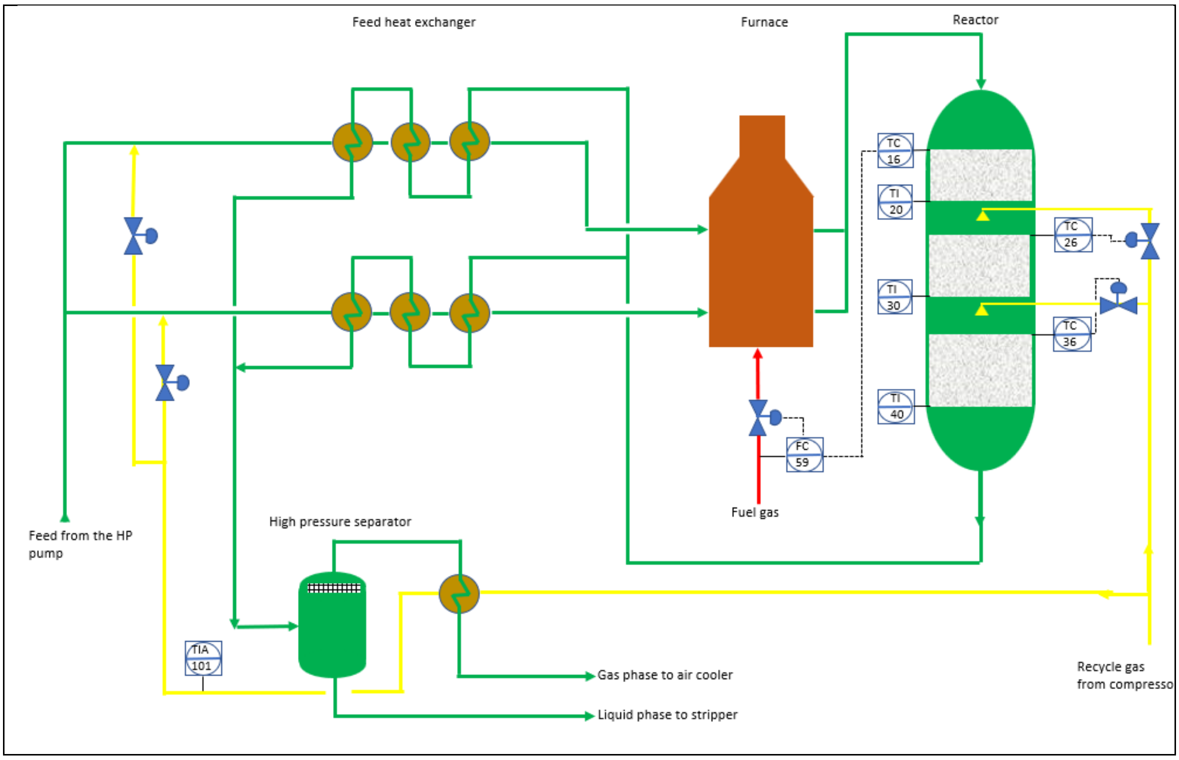


Figure 39 Simplified flow diagram of hydrotreating reactor process

The hydrotreating process, which is related to this thesis, is presented in Figure 39. The flow diagram is simplified, and only the relevant measurements, process lines and equipment are presented in the figure. The feed section, compressors and separation process after the high-pressure separator are not shown.

Feed from the feed drum is pumped at high pressure through a heat exchanger train into the furnace. The hydrogen from the recycle gas compressor is mixed with the feed before the heat exchangers. This hydrogen stream is needed for the hydrotreating processes and is the only hydrogen source for the first catalyst bed. On the other side of the feed heat exchangers flows the reactor effluent coming out from the reactor. This stream is cooled and releases heat for the feed stream.

The preheated feed continues into the furnace, which heats the feed to the heat level needed for the hydrotreating reactions. The furnace has burners at the bottom, and feed flows inside the furnace in multiple coils. The furnace uses refinery fuel gas as the energy source, and the temperature controller TC16, which controls the first-bed inlet temperature, sets a remote setpoint for the fuel gas flow controller FC59.

The reactor has three catalyst beds; the first-bed catalyst proportion is ~18%, the second ~39% and the third 43% of the total catalyst mass.

The second-bed inlet temperature is controlled by TC26, which uses hydrogen quench as the cooling media. This hydrogen quench is coming from the same recycle gas compressor as the hydrogen flow into the feed stream. Cool hydrogen quenches reduce the temperature that is increased in the exothermic processes. The third bed inlet temperature is controlled by TC36, and functionality is like TC26.

After the reactor, the reactor effluent flows through the heat exchangers into the high-pressure separator, where the first separation of the gas phase and liquid phase occurs. The gas phase continues into the cooling phase and finally back into the recycle gas stream. The liquid phase continues to the stripping/distillation separation process.

9.2 APC reactor design

As the controller was planned to be implemented as in-house work as thesis work, the related costs are small, so no formal gate approval process was needed. The need for the controller was raised in the operations organisation, and the expectation is that it will ease operator work and control reactor temperature better in constrained situations.

It is impossible to estimate benefits from this specific APC controller, as the reduced temperature fluctuations and better operationality in constrained situations will not automatically lead to economic benefits, or they are challenging to estimate and calculate. The controller is a tool for the operator to control reactor temperature and catalyst bed temperature distribution more accurately than manual operation. After the controller is commissioned, comparing process data before and after commissioning can be done and possible benefits can be estimated from the actual process data.

As the biobased feed that is planned to be fed into the reactor has not been started yet at the time the controller is designed and commissioned, the possible limitations in the reactor section are not known. Biobased feed will increase the exothermic reactions in the reactor, oxygen removal reactions are one significant change compared to fossil-based feed. For reactor temperature controllers, it will mean reduced fuel gas consumption in the furnace and increased quench hydrogen flow to catalyst beds 2 and 3. MPC-controller will be the tool to operate the reactor efficiently in this new operation mode and reduce the need for operator manual DCS temperature controller setpoint operations.

After plans and discussion with the operations and process engineer, the following controller structure was decided.

9.3 NAPCON

NAPCON is a business unit of Neste, and the NAPCONs product portfolio consists of multiple industry digitalisation tools, like process information system NAPCON INFORMER, data analysis tools NAPCON ANALYTICS to visualise real-time KPI dashboard to ease human decision making. Operator training simulator, NAPCON SIMULATOR, is an efficient tool to train operations personnel to operate the process units in different situations like process upsets and other demanding operations. Advanced control systems can, in some cases, minimise the need for manual operations, and at least for the new operations personnel, the real hands-on experience of how to operate the unit in unordinary situations can be difficult and slow to achieve. With a training simulator that is modelled to mimic the real process unit behaviour as closely as possible, the training of new skills and maintaining the competence level is an powerful and very cost-efficient method.

NAPCON CONTROLLER, OPTIMIZER and ADVISOR COLUMN belong to the NAPCON improve products. Optimizer is based on dynamic real-time optimisation concept and can be used on the optimisation layer above the MPC controllers. Advisor column is an AI solution that works as an AI assistant for operators and engineers related to crude oil distillation operations (Napconsuite). NAPCON controller is an efficient MPC controller that was selected as the technology for this reactor MPC controller.

9.3.1 NAPCON CONTROLLER

NAPCON controller is a flexible controller that can be used from small to large applications. It can be used to handle linear and non-linear processes and efficient optimisation algorithms allow fast only few seconds control cycles (NAPCON technical brochure).

This reactor controller will be running at 60-second intervals, as the process response is also relatively slow, and faster control would not increase the performance.

The controller software package includes the NAPCON INFORMER, which is used as the database for the controller and the NAPCON MODELLER for the modelling phase. Simulation software is also included, which is used to operate the controller in simulated mode to perform initial tuning, and NAPCON Improve Operator Interface is used to configure the operator visual user interface.

9.3.2 Process information system

The site uses ABBs Windows-based process information system that consists of Real Time Database (RTDB) and Vtrin user interface (ABB Oy, 2019). The process information system combines the process data from several separate DCS systems, and an efficient database enhances good trending tools for process monitoring. The system also has some APC-related functions integrated, and communication between the DCS and APC layer is done via this system, increasing its functionalities wider than in a traditional process information system.

9.4 Controlled variables

9.4.1 Weighted Average Bed Catalyst Temperature, WABT

WABT is the most important controlled variable, as it presents the whole reactor temperature and can be used to set and keep the desired level of reactions. WABT was already calculated in the DCS system, so no new calculation was configured for the APC. WABT is defined as a target-type CV.

Current DCS calculation uses the simple Equation (1) to calculate the bed WABT, not the version that would give more weight to the outlet temperature (2).

$$WABT = \frac{T_{in} + 2T_{out}}{2} \tag{1}$$

$$WABT2 = \frac{T_{in} + 2T_{out}}{3} \tag{2}$$

The WABT calculations use median temperature values, Figure 40 shows second bed outlet temperatures during 90-hour period. Feed quality and temperature setpoint changes are common in this process unit. The three temperature measurements in the diagram are at the same level in the catalyst at a 120-degree difference, so they should all read the same temperature. There is usually some level of difference in the outlet temperatures, which can be caused e.g. by differences in liquid/gas distribution through the catalyst bed and how they change during normal operations.

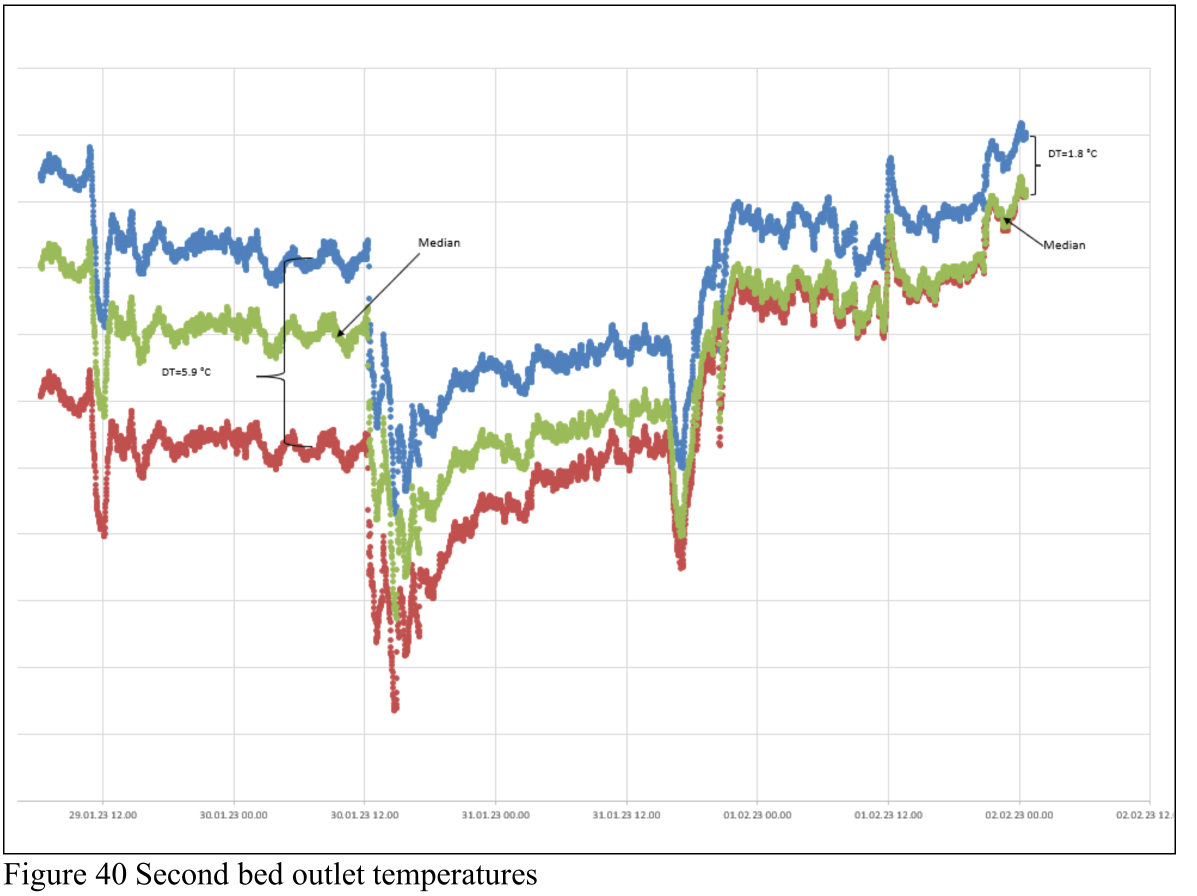


Figure 40 Second bed outlet temperatures

The temperature marked with green colour has been the median temperature in this data period; in some points, it has been clearly between blue and red temperatures, and very close to red temperature on other points. Using the average of these temperatures could improve the current WABT calculation on some level, but not much, as can be seen in Figure 41, which presents different calculated WABT versions from a more extended time zone.

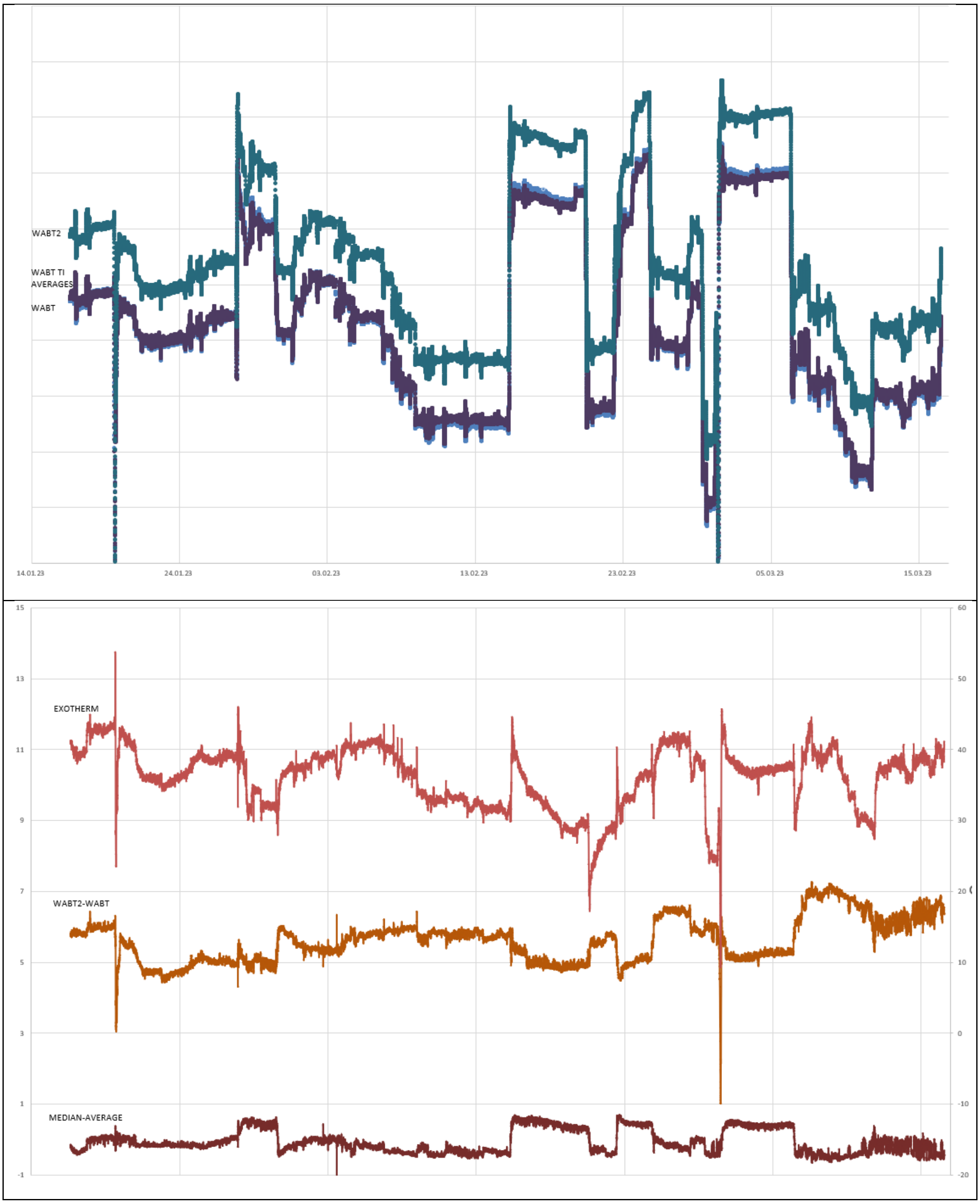


Figure 41 WABT calculation versions and the results

The current WABT (blue line), which is in use in the automation system, and the same calculation using average temperatures (light blue) have a quite a small difference; the average difference was -0.06 °C. Between the WABT2, which is calculated using Equation 1, and the current WABT, the difference is more significant as the average difference was

5.6 °C. Exotherm (red line), the ΔT between catalyst bed inlet and outlet expresses the amount of catalytic reactions, and from the trends, it can be seen that in the area of higher exotherm, the difference between WABT2 and WABT increases. This can be explained by the nonlinear temperature profile in the catalyst bed, and it can be expected that in higher activity, the temperature increase is larger in the lower catalyst bed part.

Table 8 WABT calculation comparison

	WABT (median-average)	WABT2-WABT
max	0.70	7.28
min	-1.06	1.02
average	-0.06	5.61

The current reactor operations are not related to the exact WABT target, which would be the same in different unit operations modes. Catalyst deactivation, changes in feed quality and changes in product specification require a change in the reactor WABT, most often based on the laboratory sample results. Replacing the current WABT calculation to use average temperatures instead of medians would not make a big difference, as seen in Table 8. WABT2 calculation would have more significant difference, and replacing the current with this should be considered. This could possibly reduce catalyst deactivation as changes in the catalyst exotherm would have a more significant impact on the WABT.

9.4.2 Reactor bed temperature balances

For catalyst beds 1-3, new balance calculations were configured. These calculate the bed outlet temperature and the deviation to all bed outlet average temperatures.

These CVs are used to control the reactor temperature profile; flat profile means all beds have the same outlet temperature; in an increasing profile, the first-bed outlet temperature is the lowest, the last the highest and in ascending profile, vice versa. These CVs are target type of CVs.

9.4.3 Bed 1-3 temperature rice

These temperature rice measurements measure the temperature difference between the catalyst bed outlet and inlet, which measures the temperature rice in the bed. A maximum limit can be set for these to keep the exotherm in the safe zone. These CVs are maximum type, and the controller will change MV setpoints only if the CV is close to or over the maximum limit.

9.4.4 Recycle gas temperature

Recycle gas temperature after heat exchanger, maximum limit can be set for the temperature. Maximum type of CV, gas temperature has maximum limit at this point of the process related to material limitations.

9.4.5 Bed 1-3 outlet temperatures

Maximum limit can be set for the catalyst bed outlet temperatures. Limits are safety limits, that will prevent too high bed outlet temperatures. Maximum type of CVs.

9.5 Manipulated variables (MVs)

Manipulated variables are the DCS controllers to which the MPC is writing setpoints. Certain constraints in the process can limit the MV setpoints. These are mentioned below each MV.

TC16, the reactor inlet temperature controller

TC16 is the reactor inlet temperature controller, that sets the temperature for the first catalyst bed. The controller is in cascade mode with furnace fuel gas flow controller FC59. TC16 is the master controller that gives a setpoint for the slave controller FC59.

Second and third bed temperature controllers TC26 and TC36 use the quench gas to control the temperature. If the first bed temperature is increased, it will cause more heat and reactions for the second bed, causing more quench gas flow to be needed for the second bed. Constraints for TC16 setpoint are:

- TC26 quench gas valve opening maximum limit. Maximum valve openings should be limited to 50% to save valve controllability, if more cooling is needed e.g. in process upset.
- TC16 controller deviation, process value (PV) – setpoint (SP). If the controller is not able to control the temperature, starts the deviation increase. Limits can be set for the deviation, which can restrict MPC controller setpoint changes.

TC26, the second bed inlet temperature controller

TC26 is controlling the inlet temperature for the second bed. Constraints for TC26 setpoint are:

- TC26 quench gas valve opening maximum limit
- TC36 quench gas valve opening maximum limit
- TC26 controller deviation

TC36, the third bed inlet temperature controller

TC36 controls the inlet temperature for the third bed. Constraints for TC36 setpoint are:

- TC36 quench gas valve opening maximum limit
- TC36 controller deviation

9.5.1 Model matrix

Table 9 Reactor controller model matrix

	TC16	TC26	TC36
WABT	+	+	+
Bed 1 balance	+	-	-
Bed 2 balance	-	+	-
Bed 3 balance	-	-	+
Bed 1 Δ T	+		
Bed 2 Δ T		+	
Bed 3 Δ T			+
Recycle gas T	+	-	-
Bed 1 outlet T	+		
Bed 2 outlet T		+	
Bed 3 outlet T			+

Table 9 presents the controller designed model matrix. The MVs are on the top row, and the CVs are on the first column. Cells with + or – sign indicate a model between MV and CV, and the gain sign positive/negative. E.g. all TC controllers and WABT have a model with positive gain. Positive gain means that increasing MV values leads to an increase in the CV value, and negative gain is the opposite: increasing MV value leads to a decreasing CV value. The accurate model information related to the gain and dynamic behaviour of CV is defined in the modelling phase.

9.6 Process testing

Process testing for model development was done for the three MVs based on the test program presented in Table 10. During the process testing, it is important that the process unit is in steady condition, with no process upsets, no change in feed quality, etc, that could disturb the response that originated from the MV move. For example, the TC16 test was performed so that the controller is in local auto- mode, and the setpoint was changed downwards 2 °C, with a wait time 2h for the process to level out, and the temperature returned to the original value. After the process was restored and all changes in the reactor section were levelled out, the test continued to the next TCs.

Table 10 Step test plan

MV		
TC16	-2 °C, keep 2 h	+2 °C, keep 2 h
TC26	-2 °C, keep 2 h	+2 °C, keep 2 h
TC36	-2 °C, keep 2 h	+2 °C, keep 2 h

Recorded process data from these process tests was used for modelling the first versions of MV/CV pairs, and step testing continued later during the implementation phase to increase the models quality.

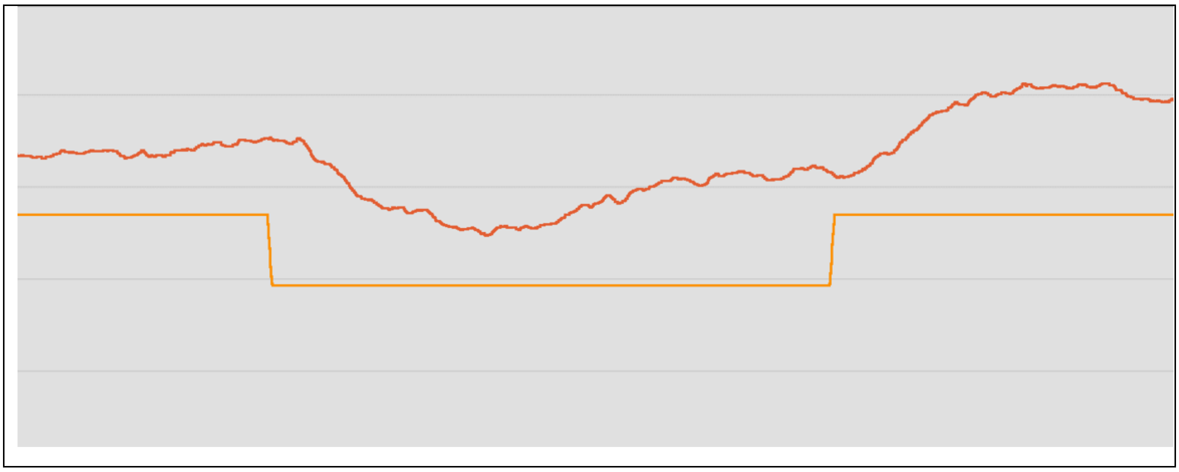


Figure 42 Process test, MV setpoint change and the CV response

One of the process tests is shown in Figure 42. The temperature controller setpoint (orange line) was first changed to 2 °C down, and after 1 hour, it was changed back to 2 °C upwards. The red line is the weighted average bed temperature. The response was not steady, and dynamic behaviour and gain were not the same in both temperature change directions. Similar problems were also present in a few other process tests. One reason is the strong interaction between catalyst bed temperatures and temperature controllers. E.g. when the first bed temperature is changed, it will change the inlet temperature to the second catalyst bed. The second bed temperature controller needs to compensate for this, changing the quench gas flow. In situations where gas flows are high and total gas flow is close to the compressor maximum, an increase in one flow controller can cause control problems in other valves (Figure 43). The recycle gas compressor is a turbo compressor, that pumps the gas with a constant rotating speed and flow, so increasing flow in one valve can cause the flow to reduce in other valves.

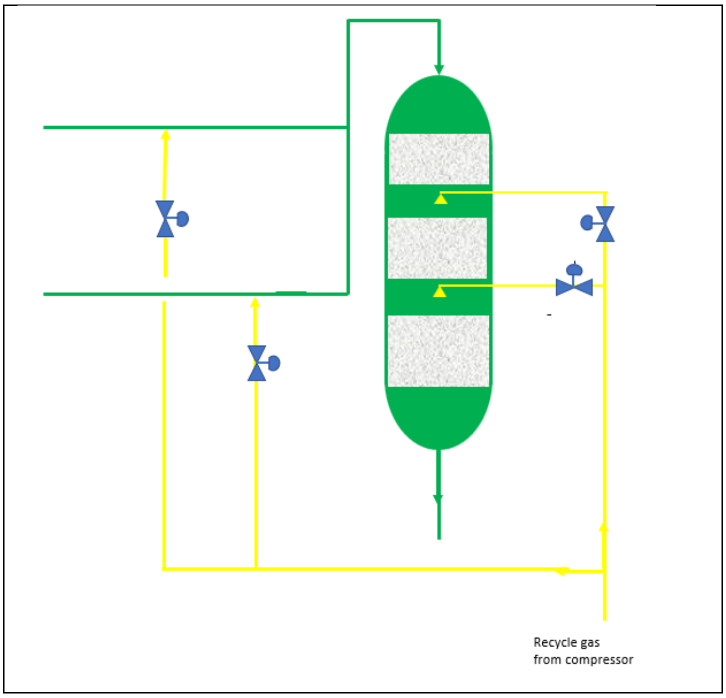


Figure 43 Recycle gas lines and valves.

Also, rector feed/outlet heat exchangers transfer the change in reactor outlet temperature to the reactor inlet. If the furnace controller cannot eliminate this entirely, it will cause an upset in reactor temperatures.

9.6.1 Modelling

NAPCON modeller software was used to develop the models. The modeller is an important component of NAPCON to improve product family, and the identified models can be used in controller or optimiser applications. The modeller fits the MV and CV process test data to transfer function models. The identified transfer models can be used to predict SISO, single input single output or MISO, and multiple input single output systems dynamic behaviour.

Typical workflow for model development using Modeller software is (Napcon Modeller User Manual 8.7):

1. Importing the data
2. Visual examination to check data quality. It is essential to check from the data that all related measurements have been working during the process test, all valves have been in the operating area, etc.
3. If needed, preprocessing of the data. For example, noisy measurements might need filtering before the data can be used.
4. Creating the model dataset by selecting the MVs and related CVs and the time range that will be used in modelling.
5. In the identification phase, modeller software generates the model. Visual validation of the model, e.g. by comparing the predicted value generated by the model and process data.
6. Model manual tuning, if needed and comparing different models to select the best model for the purpose.
7. Exporting the model to the controller software.

The identified model between temperature controller TC16 and WABT is shown in Figure 44 a-d.

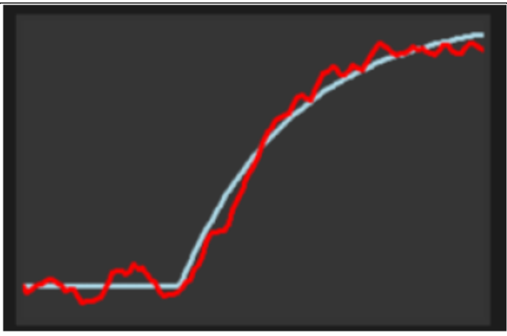
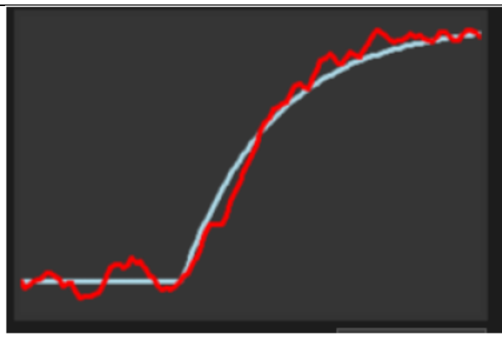
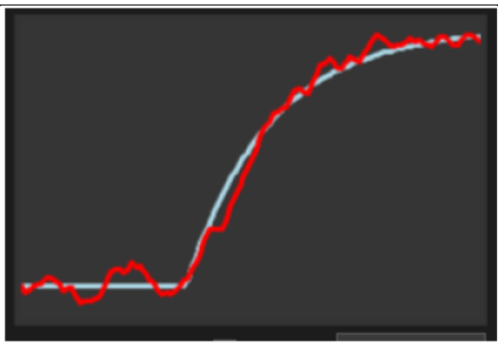
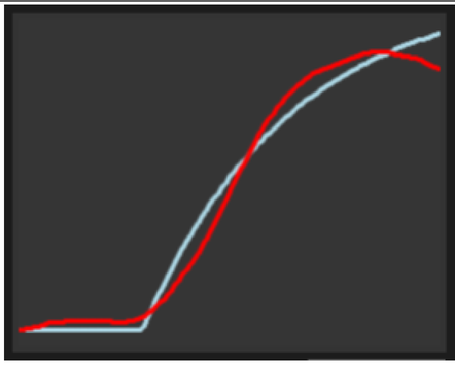
 a) Gain 0.54, T_1 26 min, DT 6 min, R^2 98,59%	 b) Gain 0.5, T_1 21 min, DT 7 min, R^2 98,63%
 c) Gain 0.5, T_1 19 min, DT 8 min, R^2 98,91%	 d) Gain 0.61, T_1 37 min, DT 1 min, R^2 98,02%

Figure 44 TC16 and WABT models.

Modelling work is often an iterative process. The first model in Figure 44 a) is the result of the Modeler tool using automatic model identification options. The blue line is the model as a first-order step response model, and the red line is the CV value. The model can be further improved if needed by manually updating model values like dead time, time constants and gain. Modelling work requires process understanding to be able to judge the model quality and to be able to select the suitable model. Process testing might need to be repeated several times to achieve good-quality process data and models.

Figure 44 b-c models the dead time, gain and time constant have been manually changed to adjust the model to match the measured process value better. No significant changes were needed, a slight improvements in gain, dead time and time constant values so that the light blue model response fits closer to the CV value. The coefficient of determination, R^2, represents the model quality. It measures how much of the dataset variation can be explained by the model, and a small improvement can be seen in the R^2 value.

Figure 44 d) the data used for modelling is preprocessed using too heavy filtering. Too large filtering smoothens the data and removes spikes, but it can also reduce the model quality as important parts of process dynamics can be lost or changed. Visually, the model and process data do not match as well as other models. The R^2 value is not a good indicator in this case; it is relatively high because the smoothed CV value has no similar spikes as the unfiltered data and the model and process data are closer to each other because of that. Also, the dead time estimation did not show correctly as the smoothened data does not have as clear a start of response as the raw data has.

The first modelling phase was done after process testing, and it took about one week to produce the needed models. During modelling, it was visible that some of the process tests required to be redone as the data from the first process testing phase was not good enough for modelling. Long delays and changes in the quench gas flows that cause disturbances in reactor temperatures were the main reasons for the insufficient quality data. The change in reactor inlet temperature took almost 3 hours before other temperature controllers reached a steady state position after the setpoint change.

9.6.2 Configuration

Controller configurations consist of communication, safety and controller functionality-related tasks. The whole control system, including the DCS, controller and needed process database functions, depends on other system configurations. Some of the required tasks related to system configurations needed in this system setup are briefly explained in this chapter.

The controller and the controller functionality-related calculation programs were built in a virtual server. A schematic picture of the software structure is presented in Figure 45. The control system consists of many separate software components, and some configuration work is needed for all of these. In this system setup, the MPC controller is not connected straight to the DCS system; there is a whole site-wide process information system that is the connection point between DCS and APC. This transfers the measured process between the systems, and calculated setpoints from the MPC are written back to DCS via the process history system.

The MPC and process history systems also have safety-related functionalities; so-called watchdog -programs follow that all needed control programs are running, setpoints are in configured operation area and setpoint changes in the control cycle are allowed sizes. Some of these functionalities are also in the DCS system to increase safety.

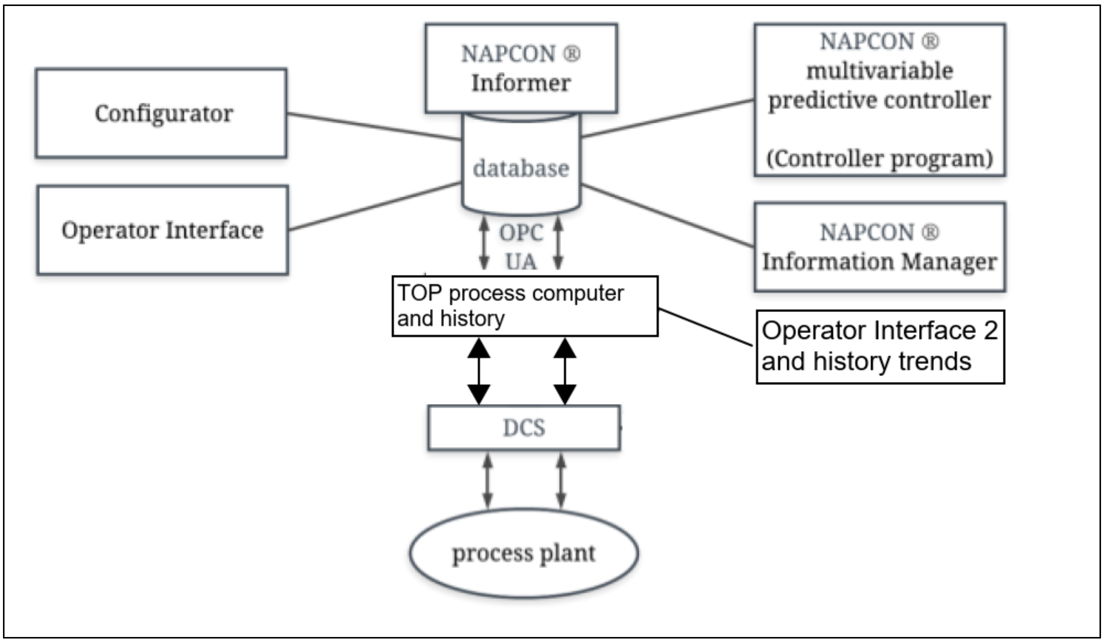


Figure 45 Schematic picture of software structure (Napcon controller reference manual 8.4, modified)

The controller user interface is Web-based and used to monitor the controller and for needed operator operations like CV and MV limits changes. The process history system also has its own user interface for APC controllers with similar functions and powerful trending functionalities.

Figure 46 Reactor controller Web-based operator interface

The operator user interface for the controller is presented in Figure 46. Operations are also possible from the process history system's controller user interface.

9.6.3 APC Controller tuning

The tuning phase is important; the controller behavior, e.g. in different constrained situations, is configured using tuning variables. This chapter presents only the basic idea of tuning and a few tuning factors. The actual tuning phase after the controller is in use can be a long work phase of up to several weeks. The controller is followed in different operation conditions and process values, and controller behavior is improved by changing the tuning.

Pre-tuning before actual controller commissioning was done using dynamic process simulation. This was an excellent way to tune, e.g. the ranking of CV steady state priorities. The importance of different CVs varies, and it is essential to prioritize the CV limits. CVs that affect process safety or controllability are more important than product qualities. For example, distillation column pressure differences are usually more important than distillate quality. Too high pressure difference over column trays can be an indication of flooding situation in the column, and product quality should be on a lower priority in the situations where controller needs first lower the pressure difference and after that control the quality CV. Low pressure difference on the other hand is not usually important, and the priority level of low limit should be low.

How the CVs are controlled when they are close or over the limit is also configured using tuning values. Around the CV limit can be defined a dead zone, where controller allows CV value to vary without controller action. Zone areas around the limits can be used to start and increase the controlling behavior before CV is on the limit.

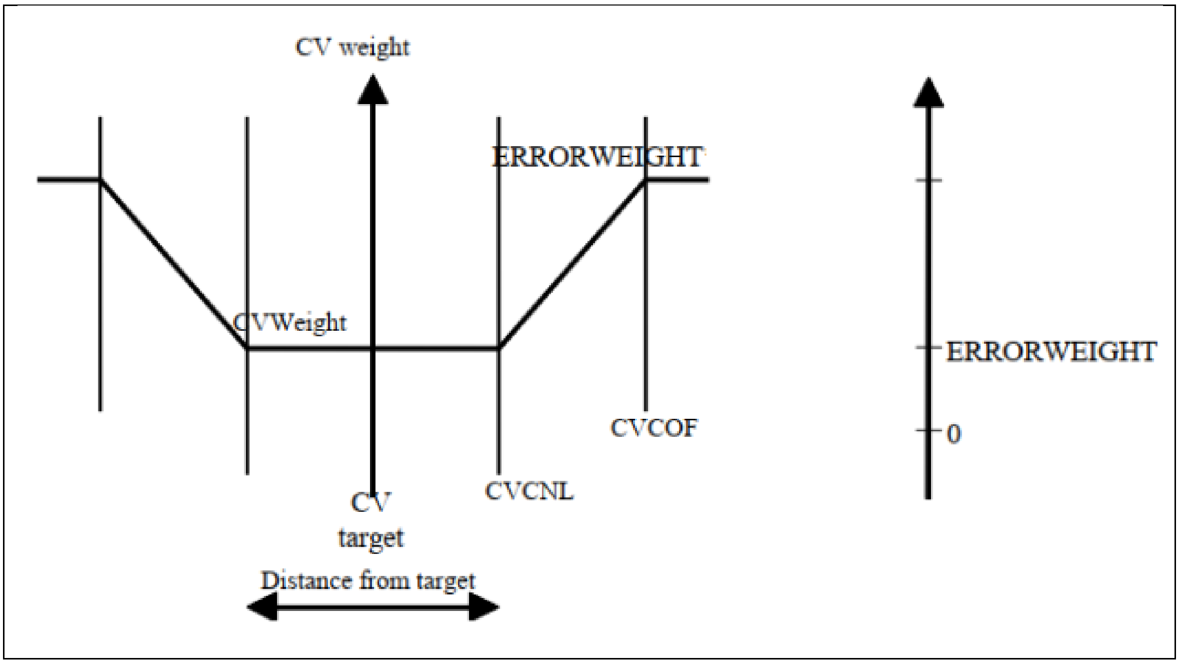


Figure 47 Symmetric CV weight (NAPCON controller reference manual 8.4)

Figure 47 presents the CV weighing around the CV target. When calculated error weight is high, the controller will do large MV movements to drive the CV to the target. The area around the limit can be asymmetric or symmetric as in Figure 47, where the CV weight is low. When the CV value goes over the CVCNL value, starts linear CV weight increment on the area between CVCNL and CVCOF. These tuning factors can affect the calm controllers actions when close to the target and be more aggressive depending on how close the CV value is to the target.

Table 11 Controller configuration and tuning variables

Control interval	Controller execution interval, often 30-60 s
Control and prediction horizon length	Depend on how long time delay between control action and the impact.
Number of calculated future control moves	Increasing the number increases CPU usage but can improve controller performance.
Scaling of variables	Scaling of different values, e.g. kg/h and t/h
CV weighting	For CV prioritizing
Move suppression	MV movement, can be used to calm MV movements.
Maximum MV movement	Maximum MV change in one control cycle
MV optimization	E.g. should MV value be maximized or minimized when possible

Table 11 lists some of the configuration and tuning variables as examples, but not all. If the process conditions or operation modes changes later, it can require new modelling and tuning work.

9.6.4 Controller commissioning

Once the pre-tuning phase was completed, the controller commissioning process was started. Using tight MV limits in the beginning, the controller was turned on, and operators were trained at the same time to use the new controller. Many of the operators were already practised operating MPC controllers in other units, so brief hands-on training in the control room was sufficient at this point. An instruction manual was written that describes the controller strategy, CV/MV variables and instructions related to starting and stopping the controller, problem-solving etc.

The controllers basic functionalities worked as planned, and after all shifts were trained, it was possible to leave the controller in control mode using normal MV limits. There was no abnormal behaviour that wrong process models or configuration errors would have caused. Small tuning changes were made to develop controller performance and to reduce small temperature fluctuations that had occurred in the beginning.

During regular steady unit operation, the controller performed at a satisfactory level. As the co-processing was not started yet during the thesis writing process, the performance in this operation mode has not yet been tested.

The processing unit is operated in many different operating modes, and related to that; the reactor temperature is often changed by several degrees in a short time. These changes are currently done using ramping functions in the DCS. The MPC is not able to make the changes as fast as the operator does them; there are more constraints that the MPC needs to take into consideration. The MPC controllers are generally tuned and designed for unit optimisations during normal operations; fast and significant target changes are generally not in the controllers scope.

Also, the DCS layer PID controllers were not fast enough to control temperatures during rapid and significant setpoint changes. Some of these problems can be fixed using more aggressive PID tuning, but some are related to limitations in quench gas availability and high compressor loading. Because of this, the controller was not used during driving mode changes. The slowness of the current PID controller behaviour decreases the APC controllers ability to control the temperatures if the feed temperature changes fast because of other operations in the unit. Some of the process models from the first process testing phase were not enough high quality because of other process disturbances at the same time. The work to develop base layer controller performance needs to continue, mainly PID tuning and operating the unit in an operation condition where the controllability of quenches remains. The modelling work needs to be redone at some level, as the change in PID controller behaviour will also affect the model dynamics.

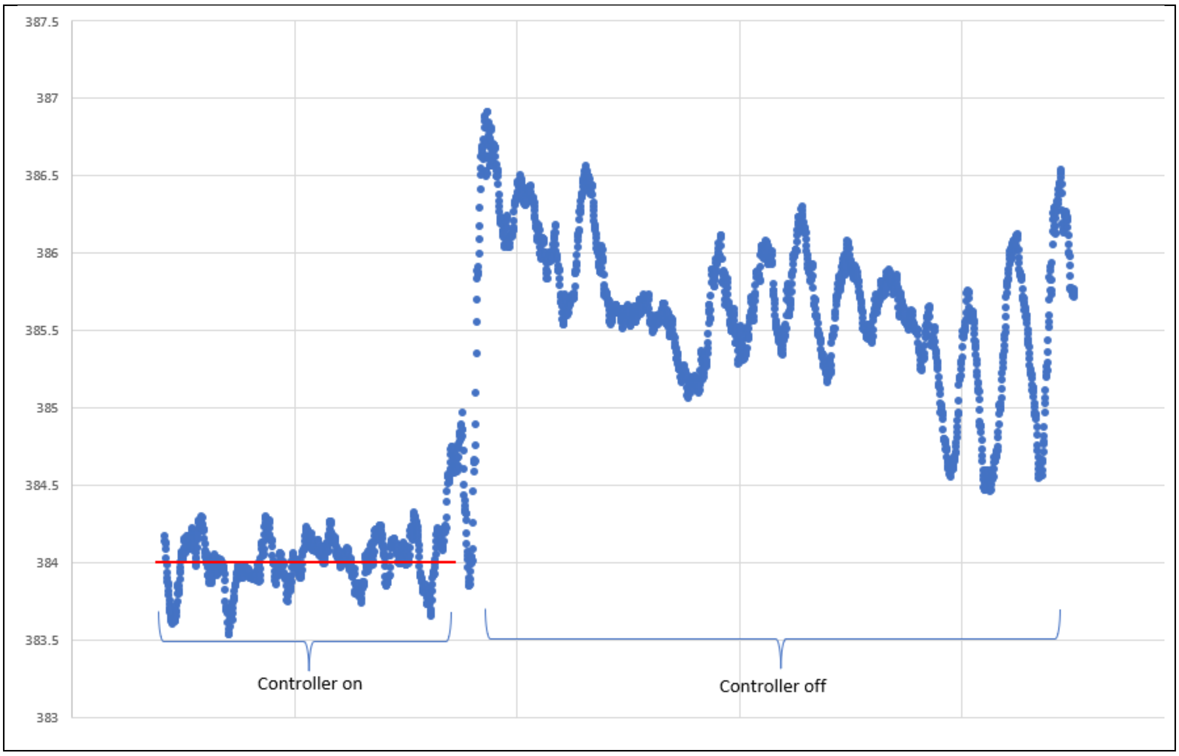


Figure 48 50 h period where the controller was on and off

Figure 48 presents one 50-hour time when the controller was in use. The blue line is the reactor WABT, and the red line is the CV target. As the controller and DCS layer PID-controller tuning were not at a satisfactory level at this controller testing phase, the controller could not control CVs with this accuracy all the time. This result still represents the accuracy increase that is possible to gain, and with more tuning and remodelling of some of the CV/MV -pairs, it should be achieved all the time when the controller is in use.

The Figure shows that when the controller was turned off, the WABT increased 2.5 °C. This is because as the controller was stopped, the MVs setpoints were also left to the last setpoint the controller had given. With more active panel operator manual setpoint operations, the temperature increase could have been minimised.

The standard deviation of the sample was calculated from this 50 h period data with Equation 11 (Nima Razei, 2023).

$$s = \sqrt{\frac{\sum(x_i - \bar{x})^2}{(n-1)}} \tag{11}$$

Where	$\bar{x}$	Mean value of the dataset
	xi	Value of i^{th} point in the dataset
	n	Sample size

The standard deviation when the controller was on is 0.25, and without the controller, it was 0.5, so it was improved by 50%, which is in line with the industrial rule of thumb that King (2011) presented: improved regulatory level control halves the standard deviation.

10 Conclusions

The controller project was an exciting learning event. After discussions with the operations personnel, the controller design was an uncomplicated task, and the design also seemed to work during and after the controller commissioning.

Limitations in current temperature controllers and significant operation mode changes were causing difficulties that I had not fully realised before commissioning. Base temperature controllers were tested at the projects beginning, but the tests were too small compared to real process changes. Relatively small changes during preliminary process testing phase gave too optimistic overall picture of temperature controllers performance, and PID tuning importance was not observed. Also, quench gas mass flow and the balance between control valves were not the same all the time, and the response and controllability varied based on the process conditions.

The old WABT calculation was also left for the controller as CV. Changing the catalyst bed inlet and outlet median to the calculated average could improve the calculation in some process conditions, and changing the equation to the version that calculates more weight for the catalyst bed outlet temperature can describe the reactions more efficiently. After finishing all other development work with the controller, the change of WABT calculation could be done. Before that, the calculation can be done as a parallel calculation to gain more data related to different operating modes.

As the co-processing of biobased feed has not started yet in this processing unit, it is impossible to calculate the APC controllers monetary value. The purpose was to improve the reactor temperature control, which would lead to the possibility to maximise the biofeed against temperature limitations.

A small improvement in temperature control and reduced WABT standard deviation, at least in some operation modes, cannot be calculated as cost-saving or other monetary value in a reliable method. Reducing temperature positively affects the catalyst life cycle, but estimating how long how long time that would be is impossible.

Improving the DCS layer temperature controller performance and MPC controller models will lead to the possibility of operating the reactor with the new controller during normal operations. When co-processing starts, some retuning and modelling might be needed. This work needs to be continued. One key learning from this project was the importance of DCS layer performance. Project work should not be rushed forward if all the necessary prework is not done efficiently and carefully.

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