Future Directions of Production Planning and Optimized Energy and Process Industries

Oil and Gas Demonstrator, TUPRAS, Turkey

Soft sensor utilization for faster characterization, physics-based and data based models, optimal control, and machine learning methods for diagnostics are used for this use case aiming at less energy use for constant quality production.

NIR soft sensor

The NIR soft sensor is developed for predicting 17 different properties of the feed simultaneously. The properties in question are:

- API
- Density (kg/m^3)
- Nitrogen (mg/kg)
- Sulphur (%)
- Distillation curve including T95. The distillation curve consists of 13 values where each point is predicted independently from each other.

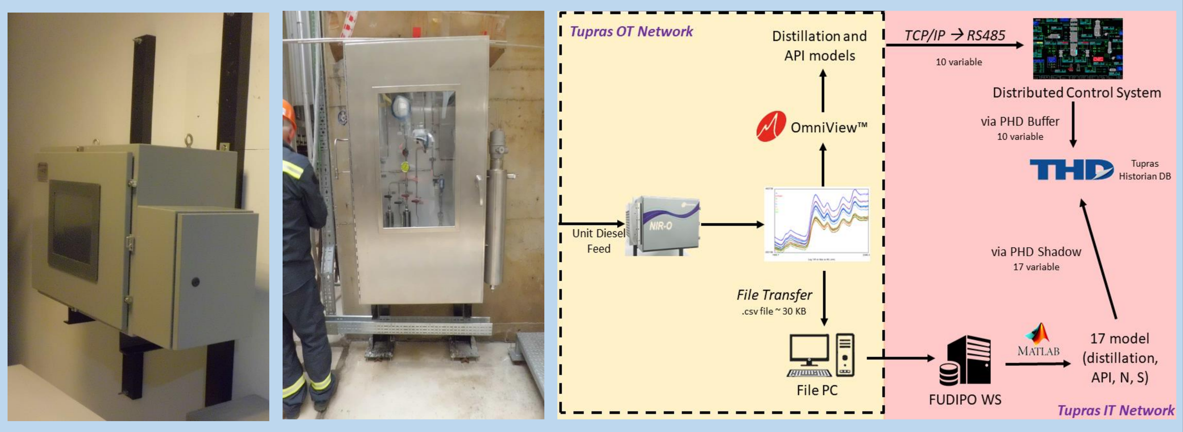

Figure 1. Online NIR analyser and preconditioning system (left) and IT/OT integration structure (right)

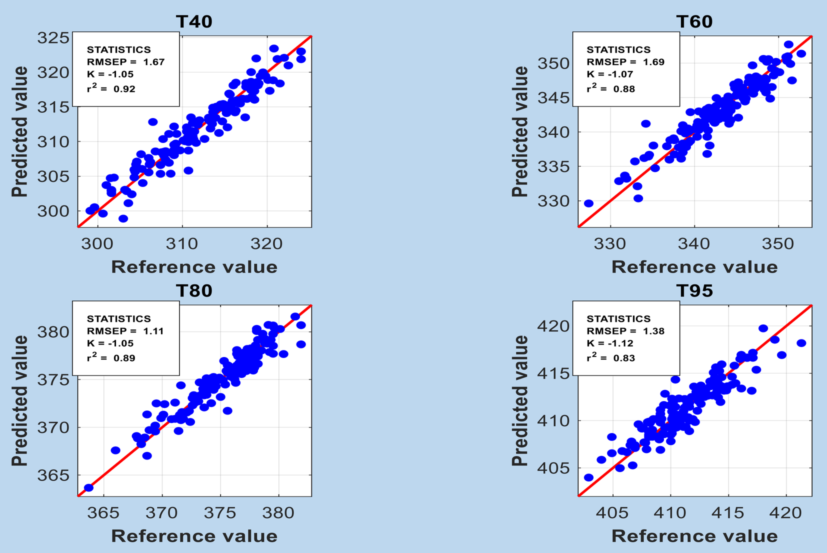

Figure 2. Estimation of feed properties based on NIR measurements

All models for all constituents are made with the same multivariate regression model technique, PLS (Partial Least Squares).

Current state: Diesel feed charging to the plant will be characterized via online NIR analyzer. Distillation points, API, sulfur and nitrogen content of the plant feed will be estimated in real time using chemometric models. Installation of the analyzer, preconditioning and recovery systems has been completed, activation and validation continue.

Expected outcome: NIR is used to detect T95 value of the feed much faster than the traditional method in use, ASTM D86. This feature enables MPC to have a feed forward structure that helps reducing the energy consumption.

Physics based models

Feed characterization

Continuous lumping approach with 161 pseudo-components is used to describe the feed. The feed lump covers the boiling range of -250ºC – 550ºC. Consecutive PCs have 5ºC TBP difference in between. Sulfur distribution is bell shaped and this is proved by the laboratory analysis of the feed mixture.

Hydrodesulfurization model

Steady-state sulphur removal reactor model is constructed and tested with an NIR input.

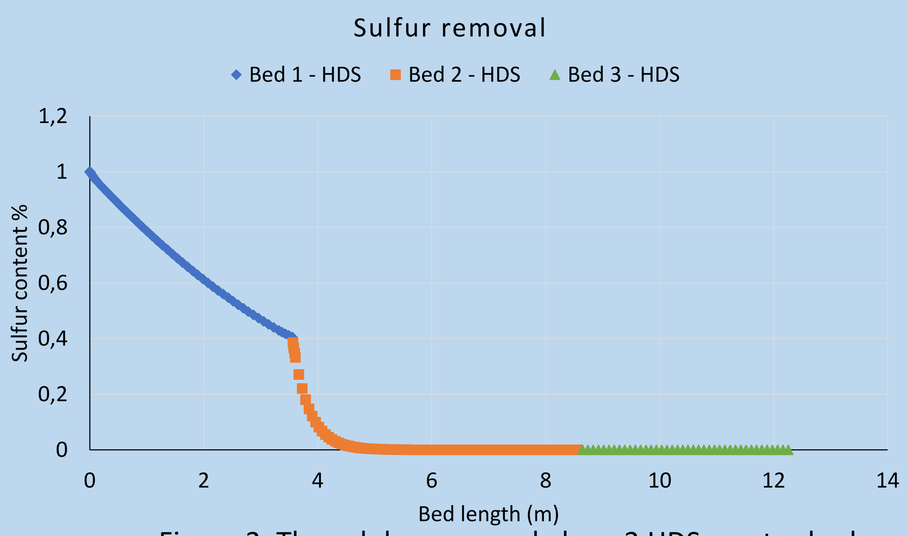

Figure 3. The sulphur removal along 3 HDS reactor beds

Hydrocracking model

Steady-state hydrocracking model is constructed and simulated with the output of the hydrodesulfurization model.

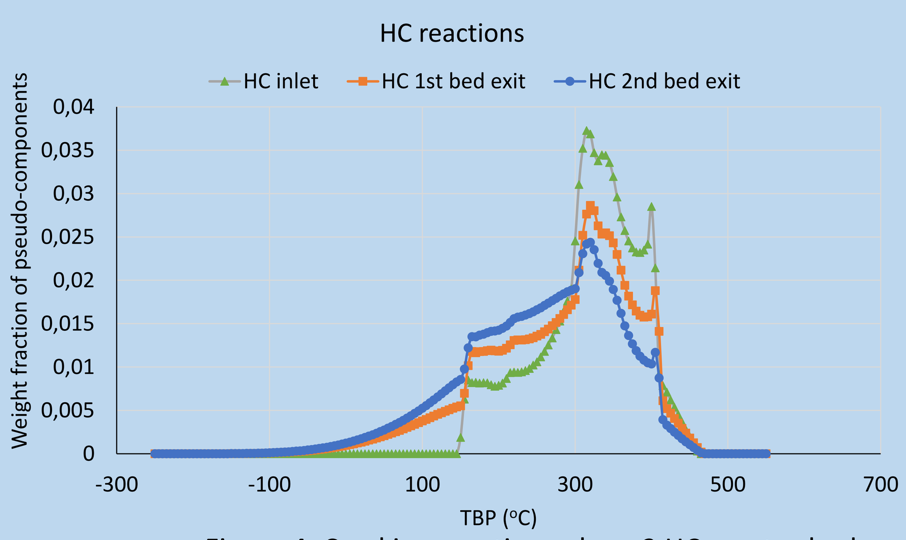

Figure 4. Cracking reactions along 2 HC reactor beds

Separation model

Column models are created on ASPEN PLUS and ASPEN PLUS DYNAMICS and the feed input is taken from the reactor simulation output.

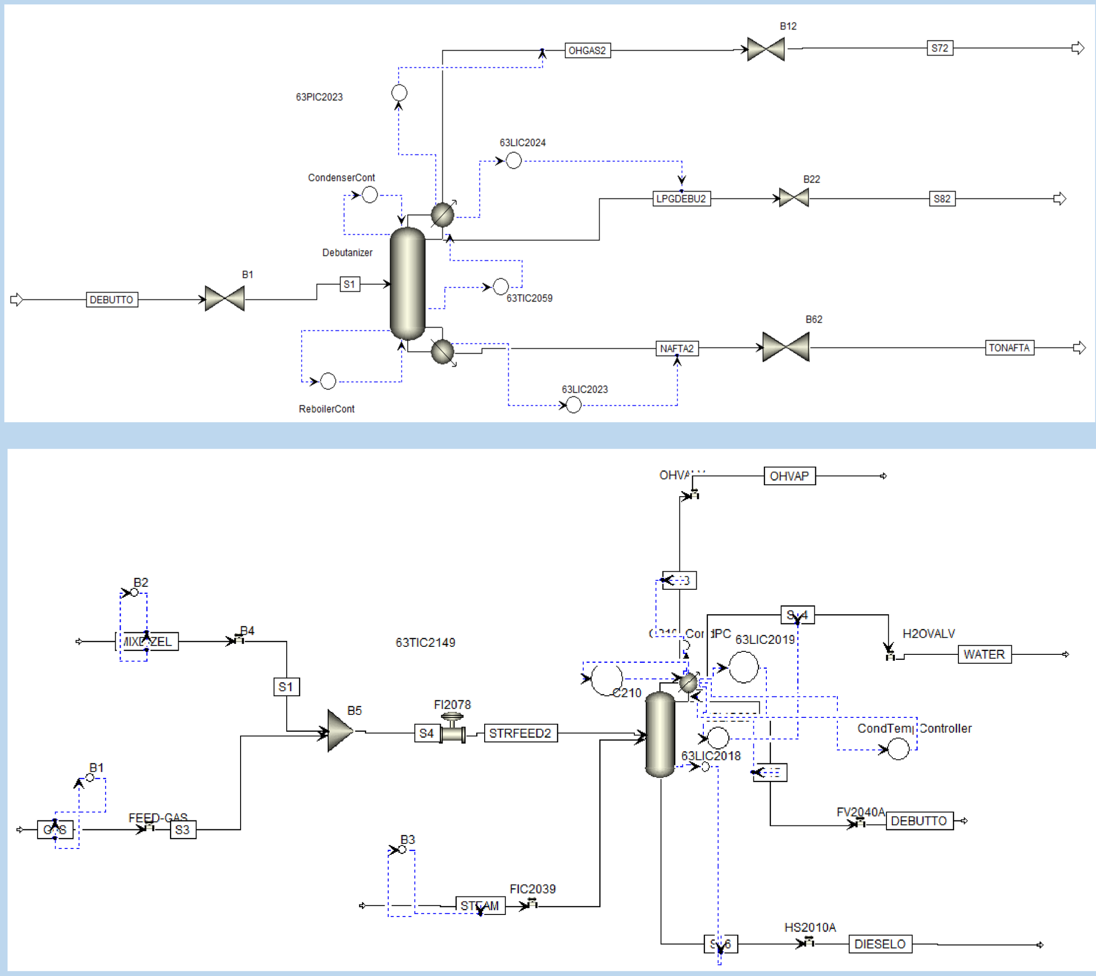

Figure 5. Separation model in Aspen HYSYS

Model testing

Model algorithm starts with the initialization step where the initial outputs (reactor effluent TBP and bed exit temperatures) are calculated; and the reactor kinetic parameters are estimated. Then by changing one system variable at once, the time variant changes in the system outputs are monitored. Dynamic model solves the mass and energy balance equations, which are differential equations with time, reactor length, and pseudo-component dependency. These equations are solved using forward-Euler method starting from the initial calculations.

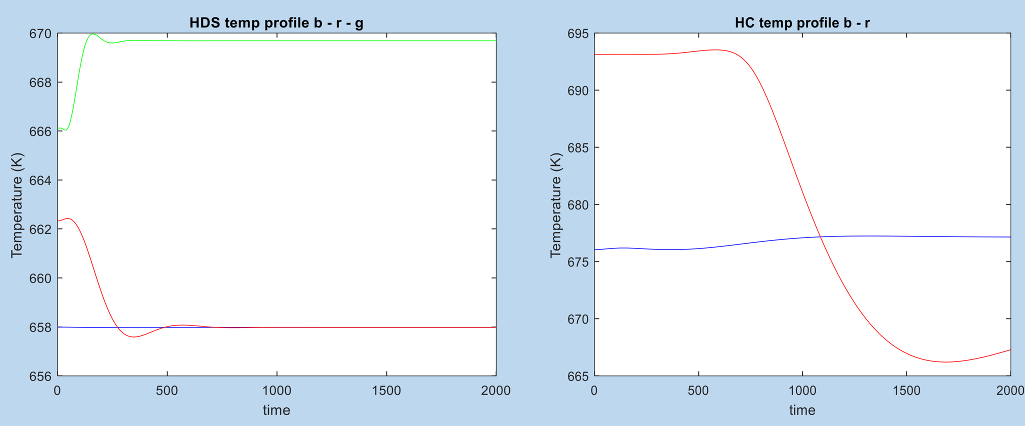

Figure 6. HDS temperature variation (left) HC temperature variation (right)

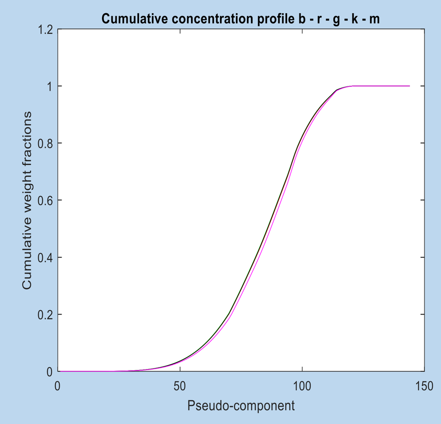

Figure 7. Change of cumulative concentration profile

The figures show that increase in temperature of bed 3, in which desulphurization reactions take place, does not have effect on product distribution. On the other hand, changes in temperatures of hydrocracking section (bed 4 and 5) cause product distribution to change. Increasing hydrocracking inlet temperatures causes the products to shift towards lighter components. Similarly, decreasing hydrocracking inlet temperatures causes decreases in rates of hydrocracking reactions, thus it causes products to be heavier.

Table 1. Comparison of the important product properties

	Simulation result	Plant measurement	Column
Diesel T95	357.9 °C	358 °C	Splitter
LPG C3/C4	0.91	0.91	Debutanizer
LSRN T95	78.20	85.30 °C	Naphtha splitter
HSRN T95	155.3	156.9 °C	Naphtha splitter

Current state: Reactor models are in Matlab environment and their steady state version is tested with the NIR input. The separation columns are steady state and dynamic but they are on Aspen Plus and to test the compatibility, Matlab output is taken as an input to this model.

Expected improvement: Dynamic models are going to be integrated to the FUDIPO Tüpraş Platform. This will enable them to integrated into live data as well.

Decision support system

Data driven models

<u>Case 1 - Quality prediction</u>

Data: 17 feed properties and process data

Prediction: Diesel product T95, Diesel product sulphur content, HSRN product T95, and LSRN product T95

<u>Case 2 - Optimization</u>

Data: 17 feed properties, remaining uncontrollable process parameters, and the targeted product quality values

Optimization: Manipulated process data (reactor inlet temperatures, temperature difference in the reactor beds, quench H2 flow etc.)

<u>Case 3 - Long-term monitoring</u>

Data: Time series analysis on process data

Estimation: Catalyst life

Table 2. RMSE of the LOO cross-validation result for labelled data

	Output Variables			
Methods	Diesel 95%	Diesel Sulfur	HSRN 95%	LSRN 95%
PMean	2.50	1.00	8.22	5.31
RIDGE	2.36	0.79	3.69	3.68
PLS	2.44	0.79	4.53	4.34
Random Forest	2.36	0.73	4.05	3.96

MPC structure

As a part of decision support system an MPC is built. For the MPC structure step test is used to build transfer functions of the plant. MPC model is on Jmodelica environment.

Dynamic reactor and separator models were developed as first-principles models using Matlab and Aspen Plus Dynamic, respectively. Then, a simplified state space model of each unit was obtained in order to develop the MPC solution. The different model adaptions which have been carried out are presented in the below scheme.

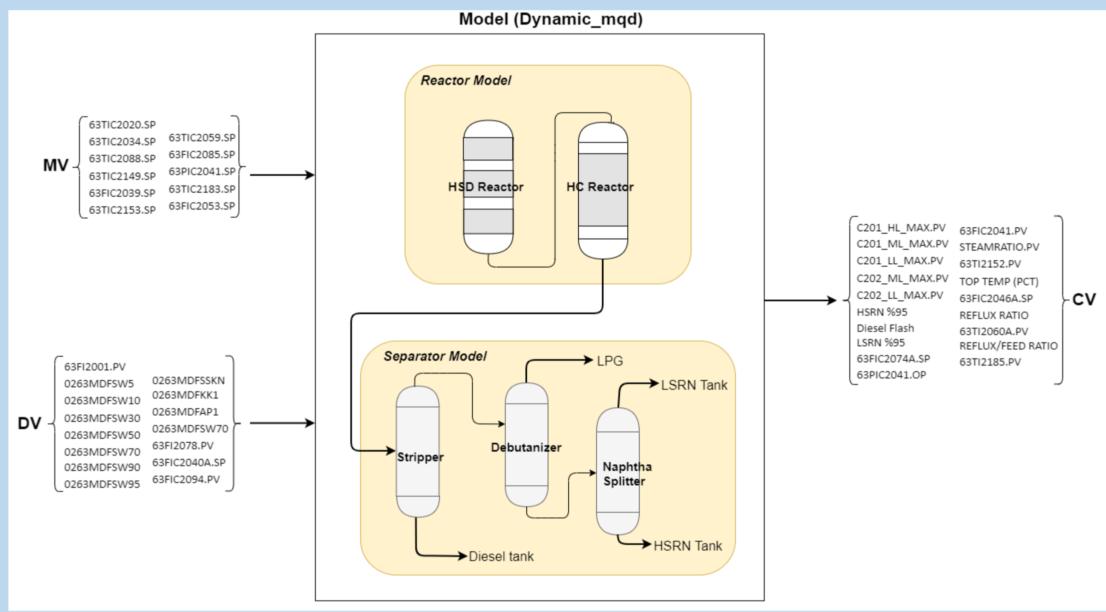

Figure 8. General model implementation scheme

Bayesian Network for Diagnostics

Case Scenario – Channelling in the reactor

Fixed bed reactors might show abnormal flow behavior and channelling in the catalyst bed is one example of it. By using the temperature measurements in the reactor, this behavior can be detected by using a Bayesian network.

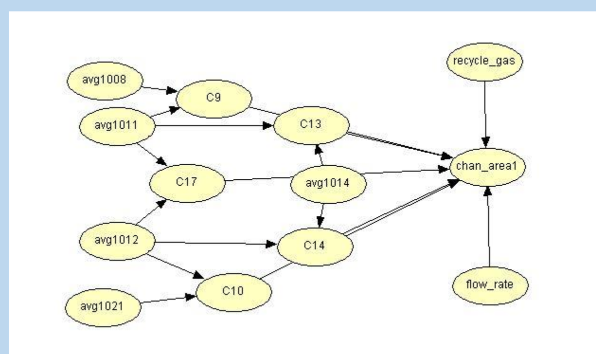

Figure 9. Comparison of neighbouring temperature sensors

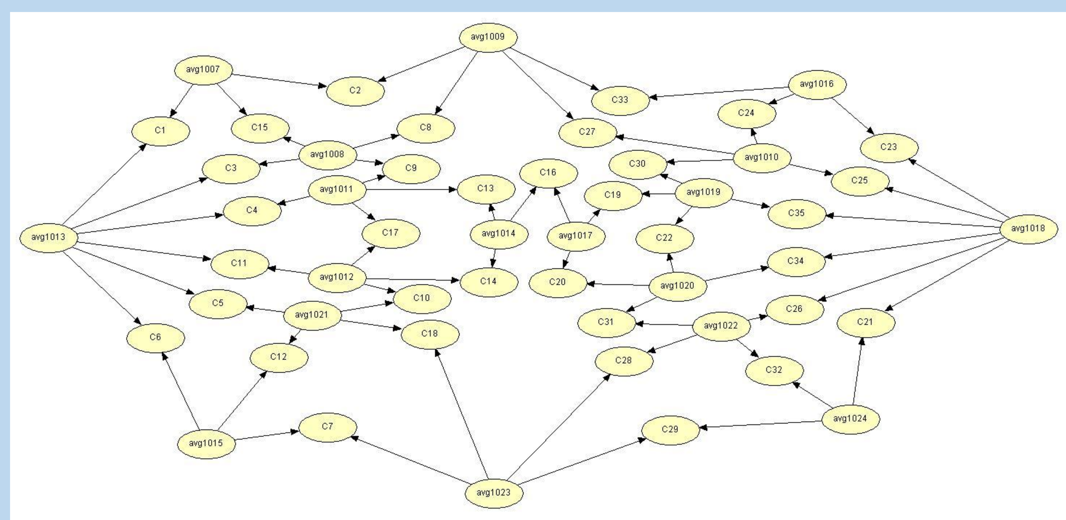

Figure 10. Map of the sensors at a certain height

Current state: Network has complicated conditional probability tables. It either needs to be filled with expert knowledge or a channeling measure has to be implemented for semi-supervised learning from data.

Expected improvement: Observing the other effects of the channeling on process values. Simplification of the network by using these process values.

This Project has received funding from the European Union's Horizon 2020 Research and Innovation Program Under Grant Agreement nº 723523