

# Future Directions of Production Planning and Optimized Energy and Process Industries

## Oil and Gas Demonstrator, TUPRAS, Turkey

Aim: Energy efficient and higher quality diesel production in TUPRAS, Izmit Refinery.

Diesel is produced in diesel hydroprocessing unit of the refinery. The unit has two reactors with total five catalyst beds. Three of these are for hydrodesulfurization and two of them are for hydrocracking. Three columns are used to separate LPG, LSRN, HSRN and diesel products.

## 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<sup>3</sup>)
- Nitrogen (mg/kg)
- Sulphur (%)

Distillation curve including T95. The distillation curve consists of 13 values where each point is predicted independently from each other.

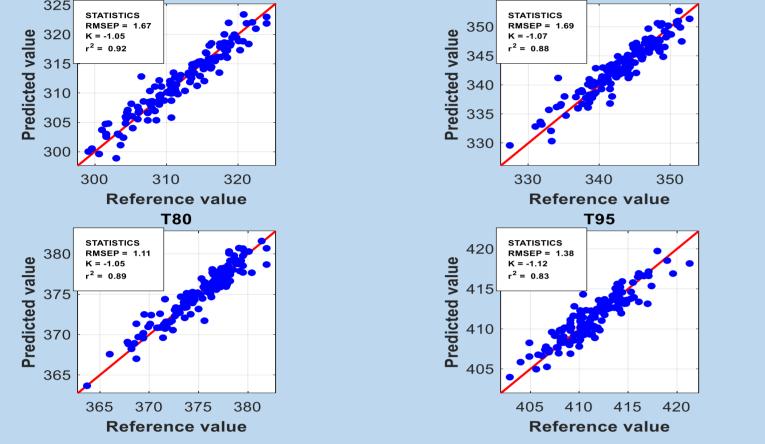
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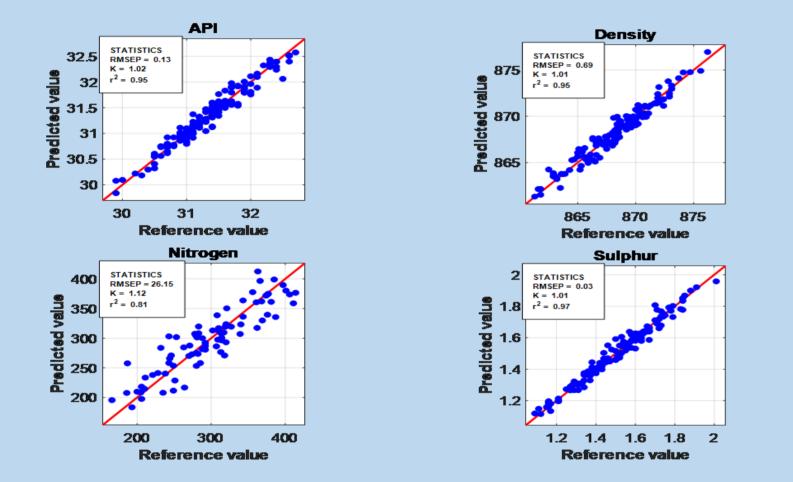


Table 2. RMSE of the LOO cross-validation result for labelled data

	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



## Figure 1. Estimation of feed properties based on NIR measurements

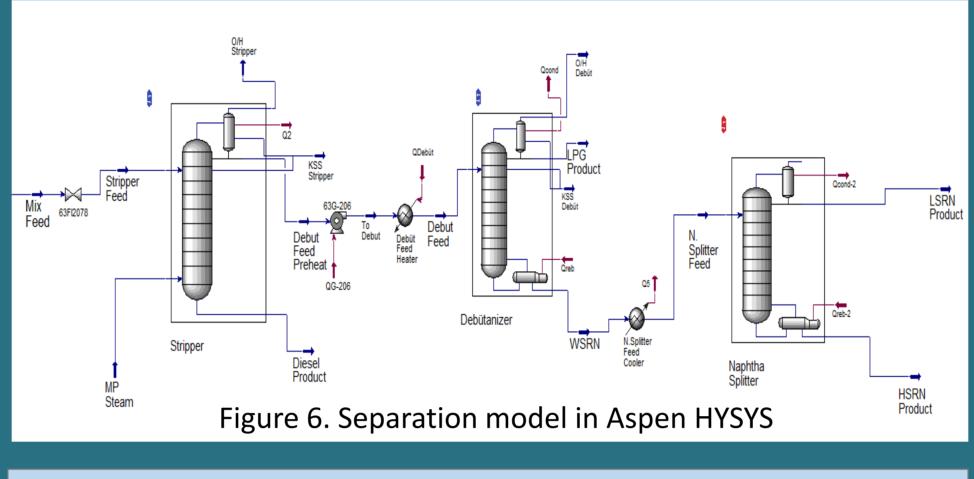


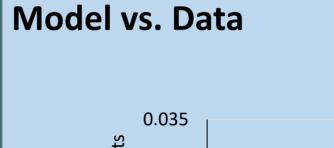
## Figure 2. Estimation of feed properties based on NIR measurements

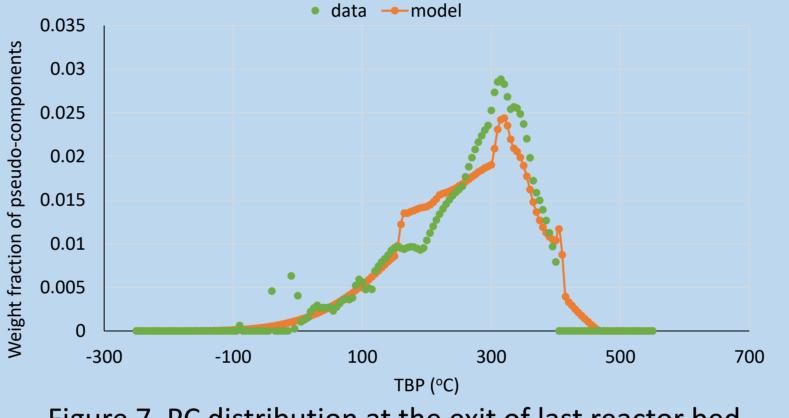
All models for all constituents are made with the same multivariate regression model technique, PLS (Partial Least Squares). **Current state:** The model development was done with collecting samples from the feed line and analyzing it with an existing offline NIR in the Tupras R&D lab. Online NIR purchasing and implementation is expected in 6 months.

#### Separation model

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







PC distribution

Figure 7. PC distribution at the exit of last reactor bed

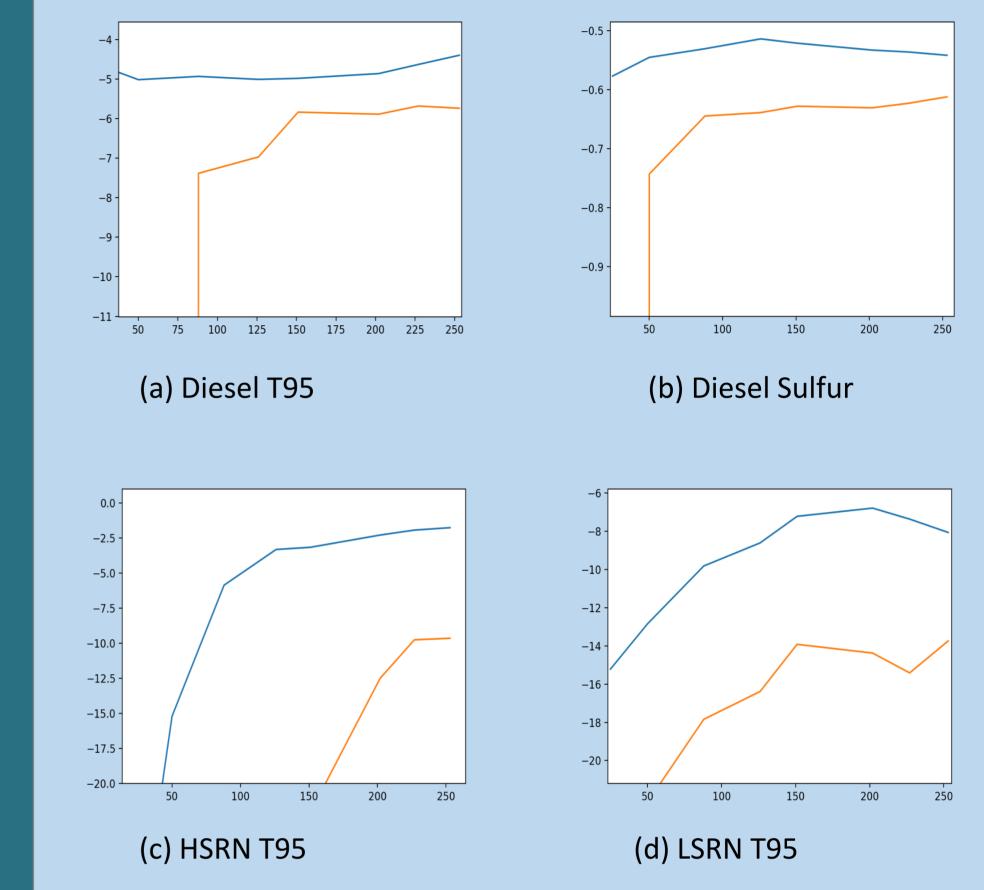


Figure 9. The learning curves for the four different output variables, showing negative mean squared error (y-axis) vs. the number training examples (days, x-axis) used for training. The upper blue curve shows the learning curve for training data and the lower orange curve shows the learning curve for the test data.

## MPC structure

**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.

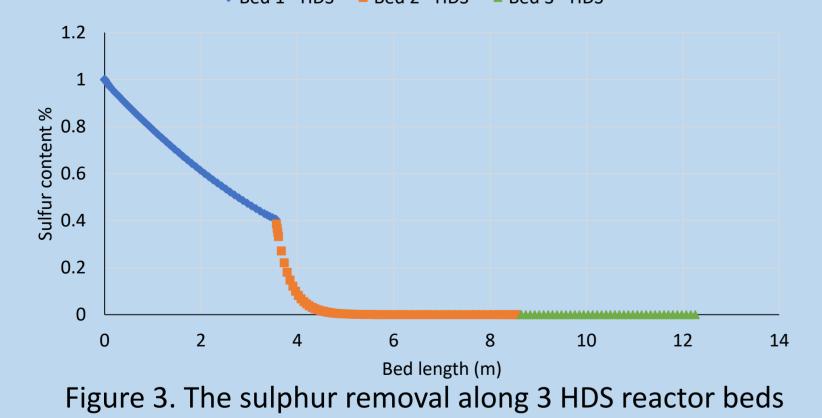
## **Physics based models** Feed characterization

Continuous lumping approach with 161 pseudo-components is used to describe the feed. The feed lump covers the boiling range of -250°C – 550°C. Consecutive PCs have 5°C 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.

Sulfur removal
 Bed 1 - HDS ■ Bed 2 - HDS ▲ Bed 3 - HDS



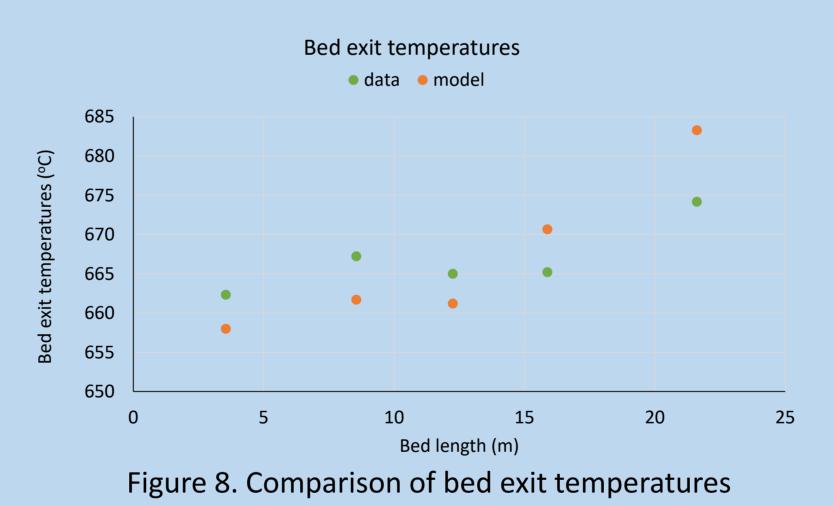


Table 1. Comparison of important product properties

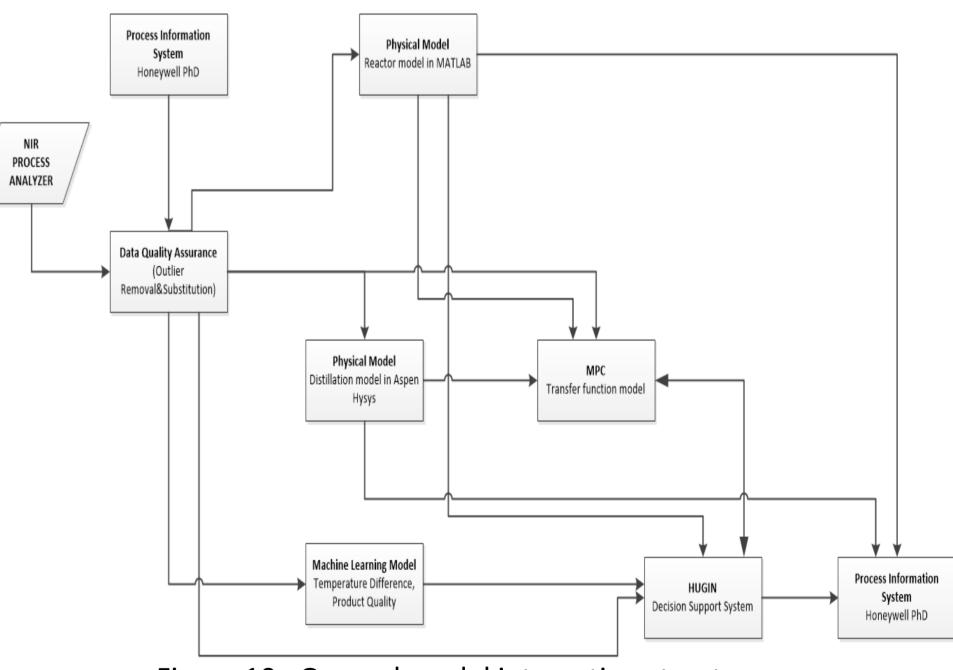
	Simulation result	Plant measurement	Column
Diesel T95	357.9 °C	358 °C	Splitter
LPG C3/C4	0.91	0.91	Debutanizer
LSRN T95	78.20	85.30 °C	Naphtha splitter
HSRN T95	155.3	156.9 °C	Naphtha splitter

Current state: Reactor models are in Matlab environment and their steady state version is tested with the NIR input. The separation columns are also steady state but they are on Aspen HYSYS and to test the compatibility, Matlab output is taken as an input to this model.
Expected improvement: For both reaction and separation parts of the system the dynamic models will be developed.

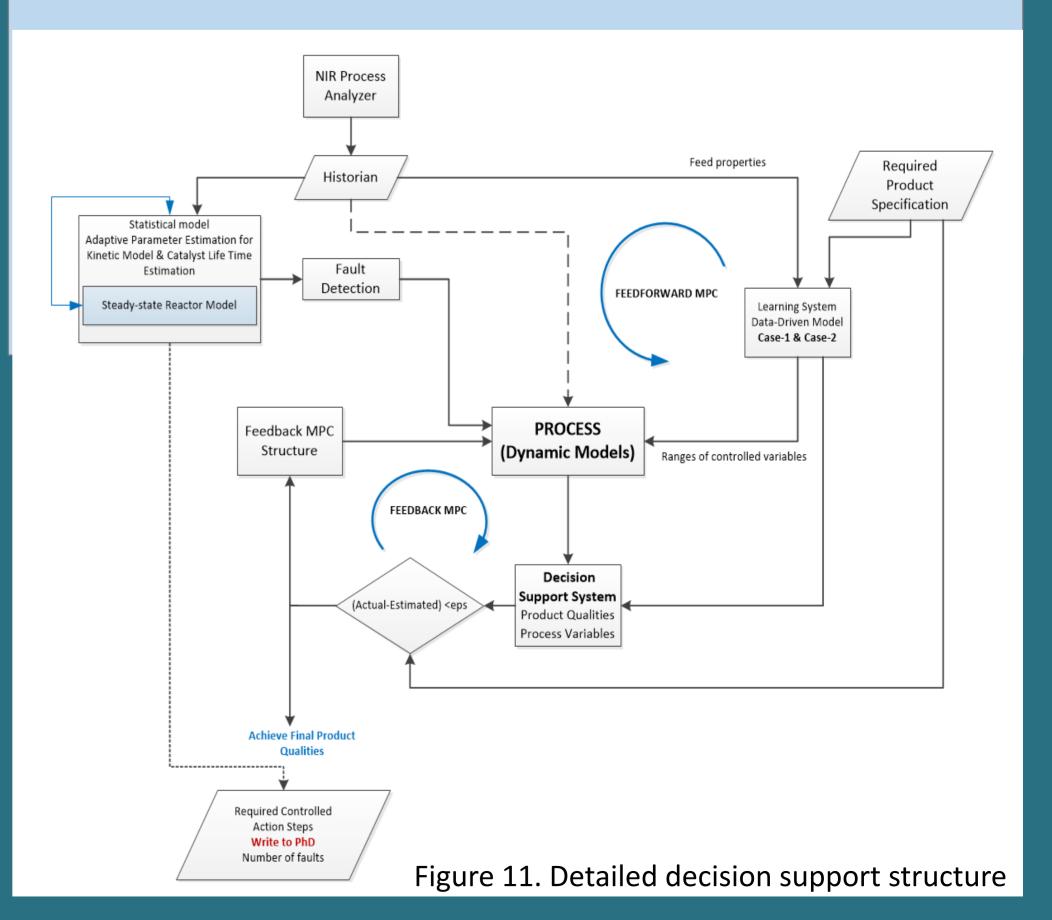
## **Decision support system**

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.

## Integration of the models

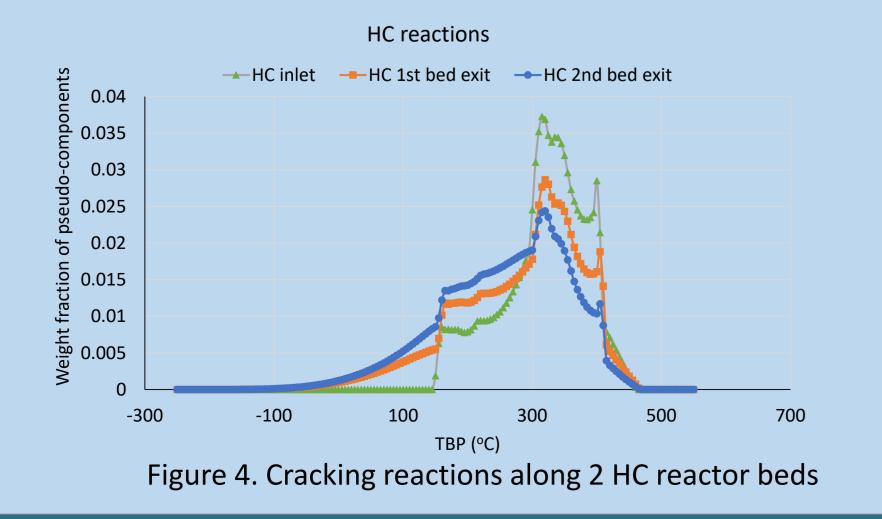






## Hydrocracking model

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



# Data driven models

Case 1 - Quality prediction Data: 17 feed properties and process data Prediction: Diesel product T95, Diesel product sulphur content, HSRN product T95, and LSRN product T95

#### Case 2 - Optimization

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 H<sub>2</sub> flow etc.)

Case 3 - Long-term monitoring Data: Time series analysis on process data Estimation: Catalyst life

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