Feedstock Characterization and Model Reformulation for SIGMA-FCC in EcoPetrol

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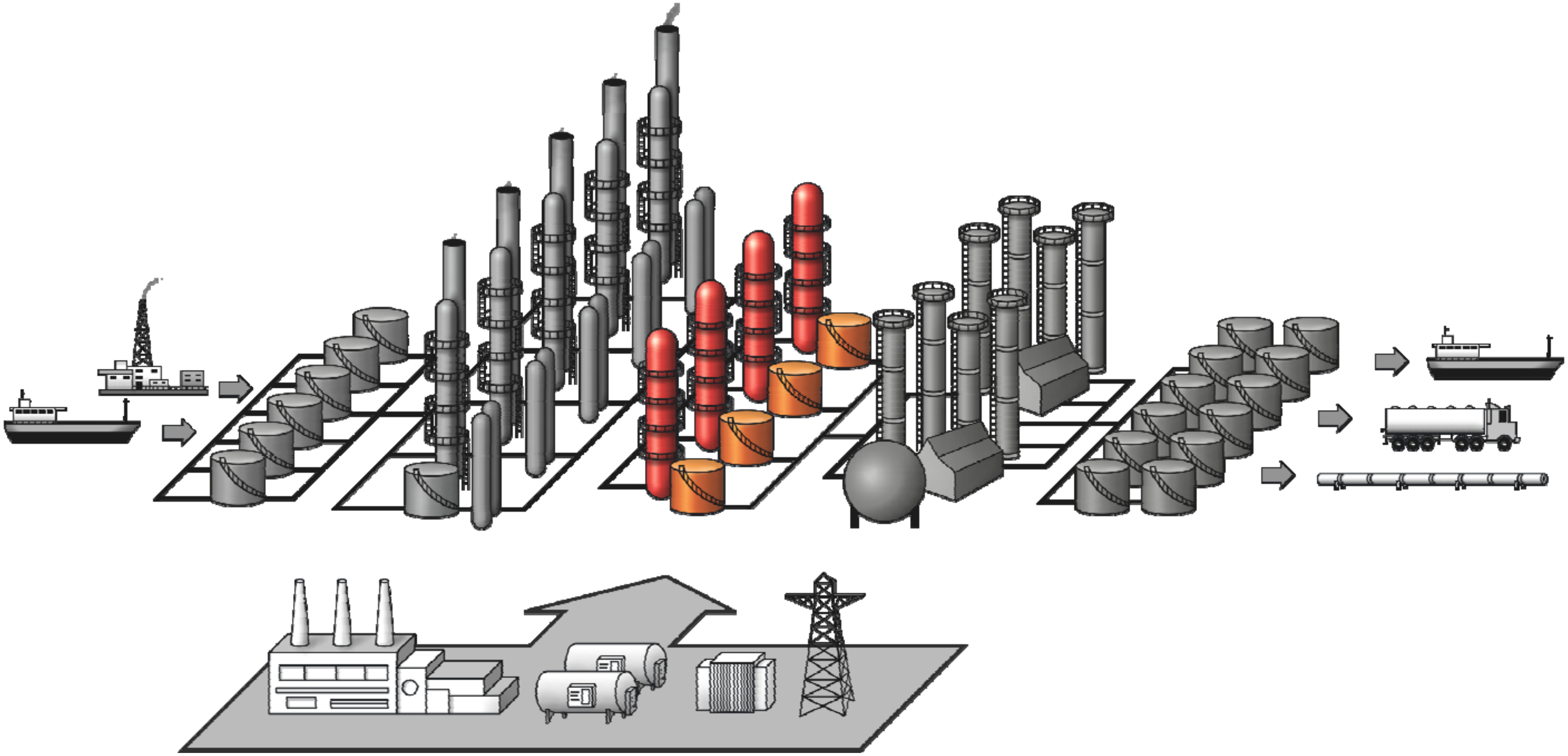
Process Landscape



Project Definition

- Two planning tools developed in EcoPetrol:
  - SIGMA-FCC
  - SIGMA-PLANNING

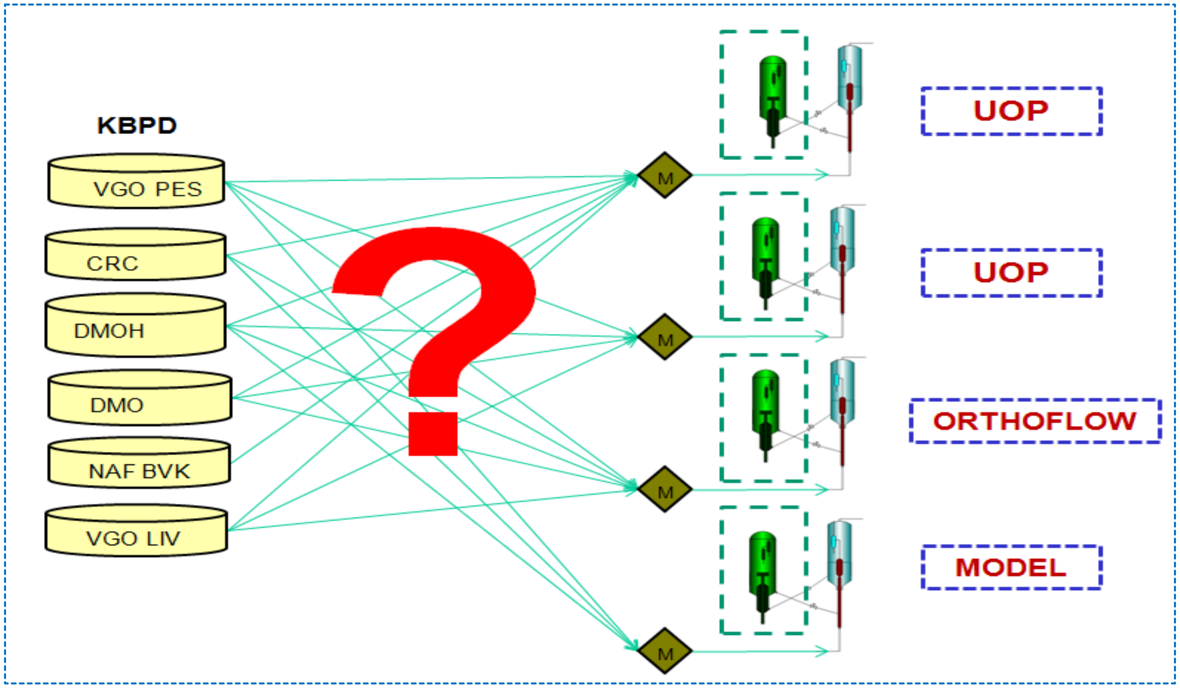
Issues:

These tools result in difficult nonlinear problems (NLP)

Tasks:

- **Reformulate the original models with advanced techniques to obtain adequate process models that cooperate with current tools**
- **Implement optimization in planning for robust convergence**

Feedstock Planning for FCC



Optimizing

Feed Allocation

$T_{preheat}$

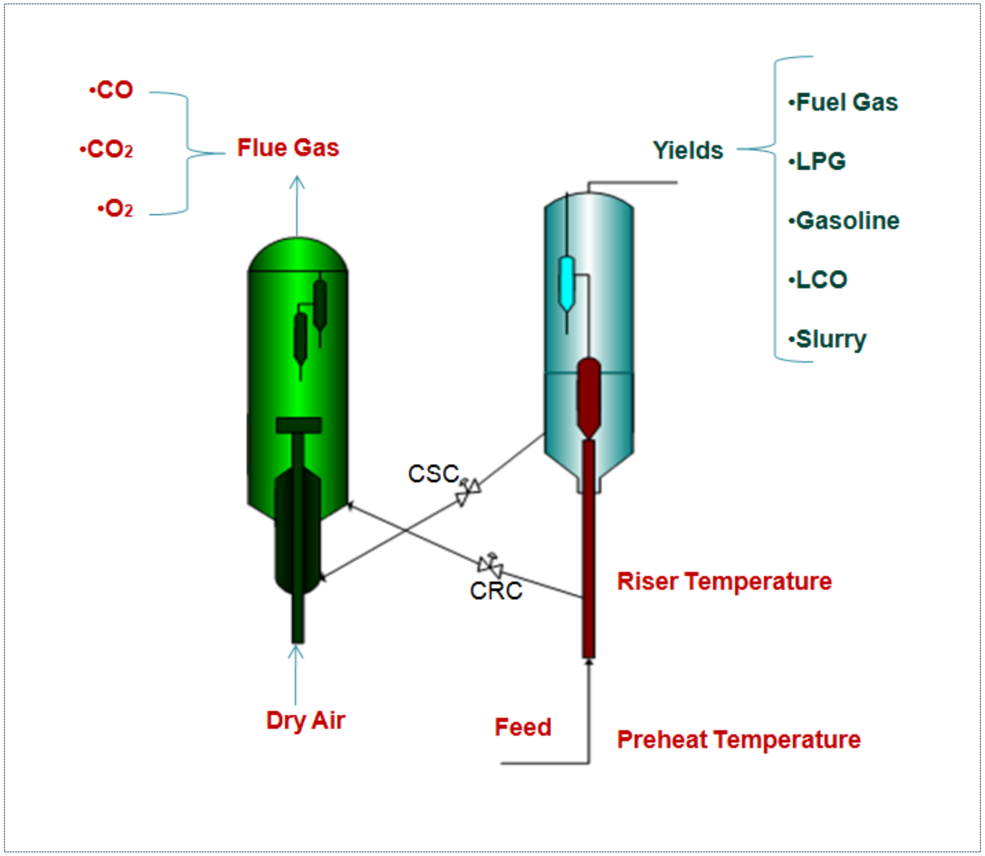
$T_{reaction}$

Maximizing Yields

or

Profit

SIGMA-FCC Planning Model



Empirical and Semi-empirical Equations.
The optimizer uses a mixed integer non-linear model (MINLP).
Solved with SBB (GAMS).

Operational Constraints

Feed availability.

Limited feed to each Unit.

Minimum and Maximum capacity for each unit.

Routing.

Minimum and Maximum riser and Preheat Temperatures.

Feed Quality Constraints

Sulphur Limit
Conradson Carbon Limit

Coke Constraints

Coke Burnt and Produced

Tuning Case

Risers and Preheat Temperature
Feedstocks
Feedstocks Properties
Products Yields and Properties
Dry Flue gas composition

Tuning Algorithm

Tuning Parameters

Simulation Case

- -Risers Temperature
- -Preheat Temperature
- -Feedstocks

Initial Conditions

- -Feedstock Properties
- -Feedstock and Products Prices

Simulator

- -Products Yields and Properties
- -Profit

Optimization Case

-Operational Constraints

-Feed Quality Constraints

-Coke Constraints

Optimizer

GAMS

- -Optimal Riser Temperature
- -Optimal Preheat Temperature
- -Optimal Feedstocks
- -Profit
- -Product Yields

**Maximize Yields
Profit**

FCC Planning Model

1. Correlations for Feedstock Properties

2. Stoichiometric Balances: Regenerator

3. Heat balance: Regenerator- Riser

4. Parameter Tuning to reproduce Riser Plant Information GRB

5. Semi-empirical Equations: Reaction chemistry kinetics in the Riser

6. Empirical Equations: Product yields

7. Correlations for Product Properties

GAMS

MINLP
Solved with SBB
(GAMS)

MODEL STATISTICS

BLOCKS OF EQUATIONS
110
SINGLE EQUATIONS
525
BLOCKS OF VARIABLES
73
SINGLE VARIABLES
371

GENERATION TIME =
0.032 SECONDS
4 Mb

EXECUTION TIME =
0.078 SECONDS
4 Mb

RESOURCE USAGE, LIMIT
0.691 1000.000

ITERATION COUNT, LIMIT
417100000

Challenges

- Complexity of empirical and semi-empirical model in EcoPetrol proprietary
- High nonlinearity of the models
- Discontinuity of the constraints
- Complementarity of the constraints
- Plan to transfer problem from discrete variables to continuous variables and solve with NLP algorithms

Complex Empirical Correlations in FCC Model

High nonlinear

- Molecular Weight $MW = f(VABP, AP, SG)$
- UOP Factor $UOPK = f(VABP, SG)$
- --- ---

Segmented Correlations

- Aniline Point $AP = f(IC, API, parameters)$
- Refractive Index $IR = f(API, parameters)$
- Basic nitrogen $N2BAC = f(API, IR, t50, parameters)$
- --- ---

Logistic constraints

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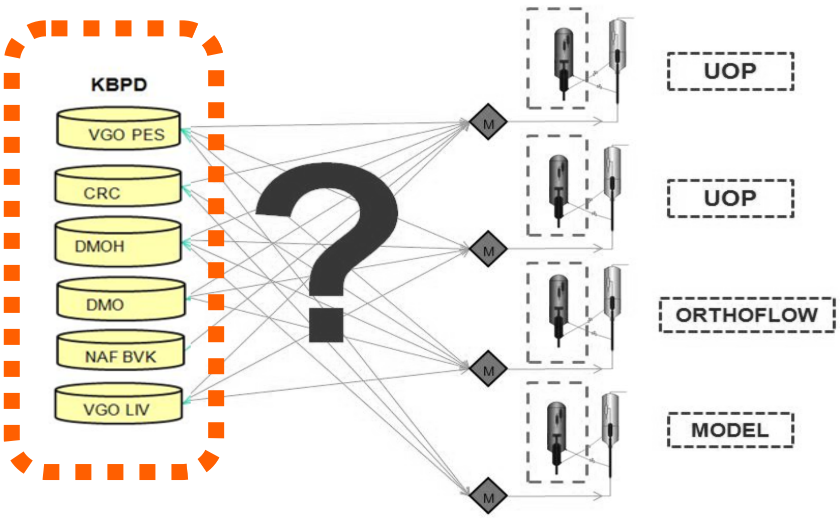
Logistic Constraints

Selecting feedstock for each unit of FCC



$$y_1 + y_2 + y_3 \leq 1$$

$$0 \leq y_1 \perp y_2 \perp y_3 \geq 0$$

$$z = f_1(x)y_1 + f_2(x)y_2 + f_3(x)y_3$$

Reformulation model

1. Linearization of highly nonlinear empirical correlation with first order Taylor approximation
2. MPCCs introduced to smooth all segmented correlation and handle logistic constraints

Results of linearization for Highly Nonlinear Correlations

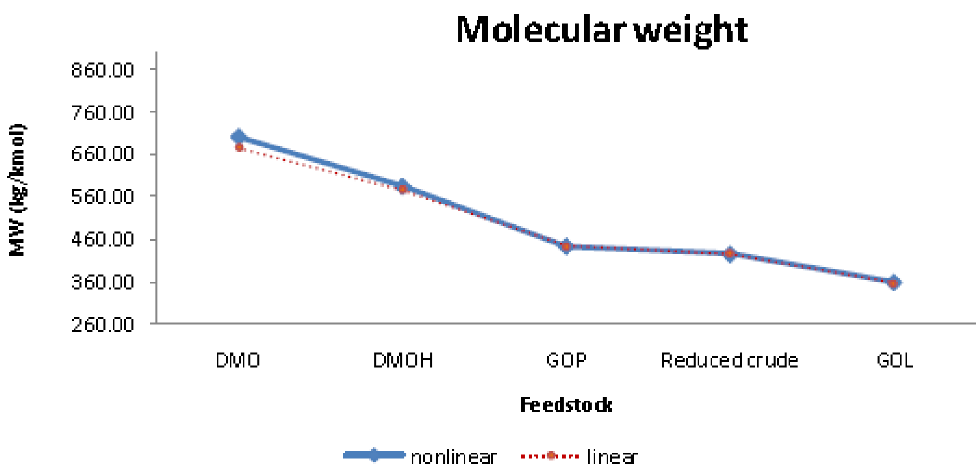


Figure A-1. Correlation for molecular weight.

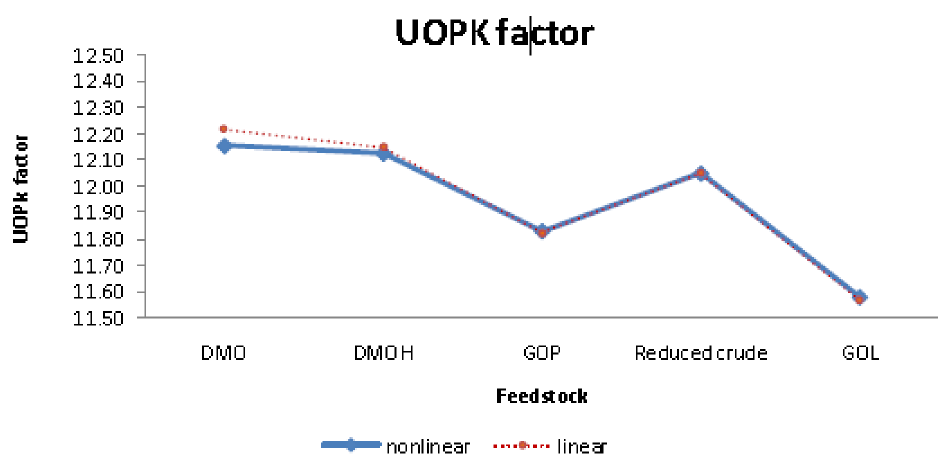


Figure A-2. Correlation for UOPk factor.

The predictions for molecular weight and UOPk factor using the linear approximation are very similar to those obtained using the nonlinear correlation.

Many others…

Mathematical Program with Complementary Constraints
MPCC

$$\begin{aligned} \min \quad & f(x,y,z) \\ s.t. \quad & h(x,y,z) = 0 \\ & g(x,y,z) \geq 0 \\ & 0 \leq x \perp y \geq 0 \end{aligned}$$

$$\Leftrightarrow \begin{cases} x_i = 0 \quad \vee \quad y_i = 0 \\ x \geq 0, y \geq 0 \end{cases}$$

$$\Leftrightarrow \begin{cases} x_i y_i = 0 \\ x \geq 0, y \geq 0 \end{cases}$$

$$\Leftrightarrow \begin{cases} x_i y_i \leq 0 \\ x \geq 0, y \geq 0 \end{cases}$$

$$\Leftrightarrow \begin{cases} x^T y \leq 0 \\ x \geq 0, y \geq 0 \end{cases}$$

Alternative for a limited class of disjunctive problems

+ can be used to model many common phenomena, including disappearance of phases, flow reversal, and hybrid dynamics
+ can embed within standard NLP solver for fast local solutions
+ Computation generally scales polynomially with problem size
- Introduces an inherent non-convexity and constraint dependency

MPCC Formulation Guidelines

- Define inner minimization problem
- Outer constraints should lead to connected regions for inner problem
- Convert MPEC to MPCC by writing out optimality conditions
- Simplify resulting expression
- Solve MPCC using NLP reformulation

Example: $y = |f(x)|$

$$max \quad f(x)v, \quad s.t. \; -1 \le v \le 1$$

$$f(x) = s_+ - s_-$$

$$-1 \le v \le 1$$

$$0 \le s_+ \perp 1 - v \ge 0$$

$$0 \le s_- \perp 1 + v \ge 0$$

$$y = f(x)v$$

$$v = -1, s_- = 0, s_+ \ge 0$$

$$v = 1, s_+ = 0, s_- \ge 0$$

$$0 \le s_- \perp s_+ \ge 0$$

$$y = s_+ + s_-$$

$$f(x) = s_+ - s_-$$

Generalized Complementarity Formulations

- Abs(*)

$$\begin{matrix} f(x) = s^+ - s^- \\ 0 \le s^+ \perp s^- \ge 0 \end{matrix} \Rightarrow |f(x)| = s^+ + s^-$$

- Min(*,*) & Max(*,*) (includes Pos(*), Neg(*))

$$\begin{aligned} & y = \min(f(x), y^{UB}) \\ & f(x) - y = s \\ & y \le y^{UB} \perp s \ge 0 \end{aligned} \qquad \begin{aligned} & y = \max(f(x), y^{LB}) \\ & f(x) - y = s \\ & y \ge y^{LB} \perp s \ge 0 \end{aligned} \qquad \begin{aligned} & Pos(f(x)) = \max(f(x), 0) \\ & Neg(f(x)) = \min(f(x), 0) \end{aligned}$$

- Signum(*)

$$signum(x) = \begin{cases} -1 & x < 0 \\ 1 & x > 0 \end{cases} \Rightarrow \begin{matrix} \min & -u * x \\ s.t. & -1 \le u \le 1 \end{matrix} \Rightarrow signum(x) = u$$

- IF-THEN-ELSE (includes Piecewise Functions but not EXOR)

$$\begin{matrix} \min & u(x - x_{switch}) \\ s.t. & 0 \le u \le 1 \end{matrix}$$

$$y = (u) f_1(x) + (1 - u) f_2(x)$$

$$\begin{aligned} & (x - x_{switch}) - \lambda_0 + \lambda_1 = 0 \\ & 0 \le \lambda_0 \perp u \ge 0 \\ & 0 \le \lambda_1 \perp (1 - u) \ge 0 \end{aligned}$$

Results of smoothing segmented correlations

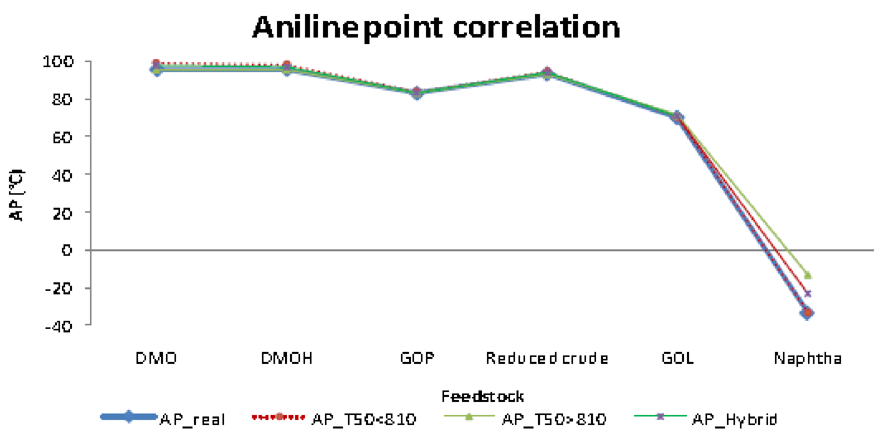


Figure B-1. Correlation for aniline point.

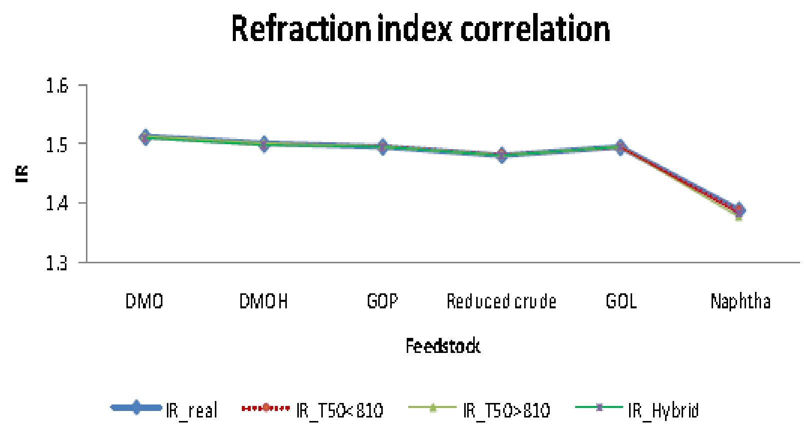


Figure B-2. Correlation for refraction index.

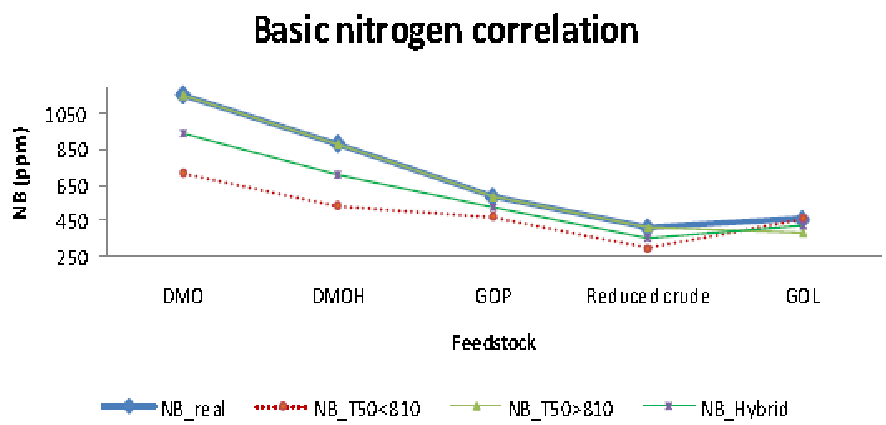


Figure B-3. Correlation for basic nitrogen.

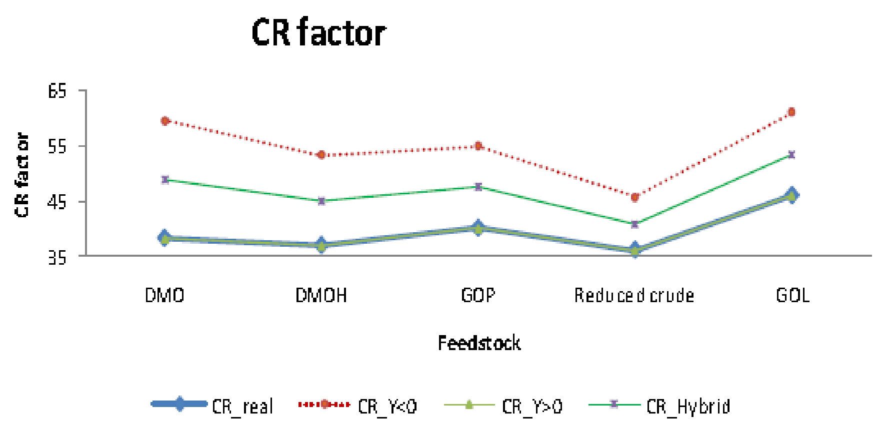


Figure B-4. Correlation for CR factor.

Results of smoothing segmented correlations (Cont'd.)

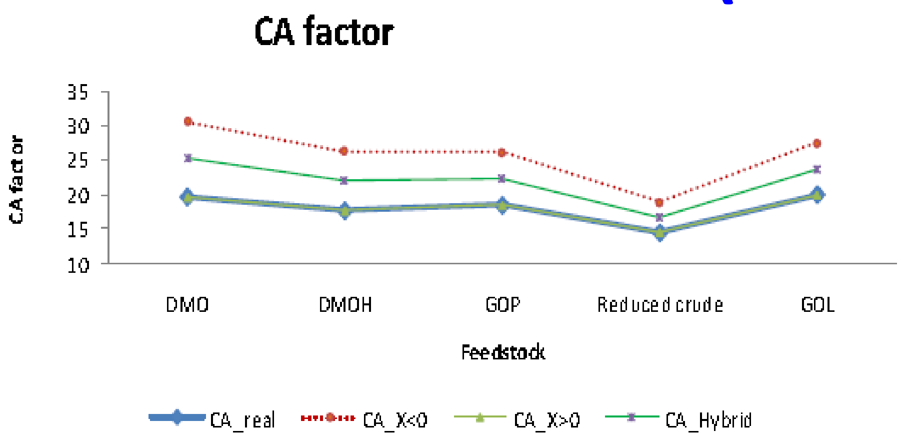


Figure B 5. Correlation for CA factor.

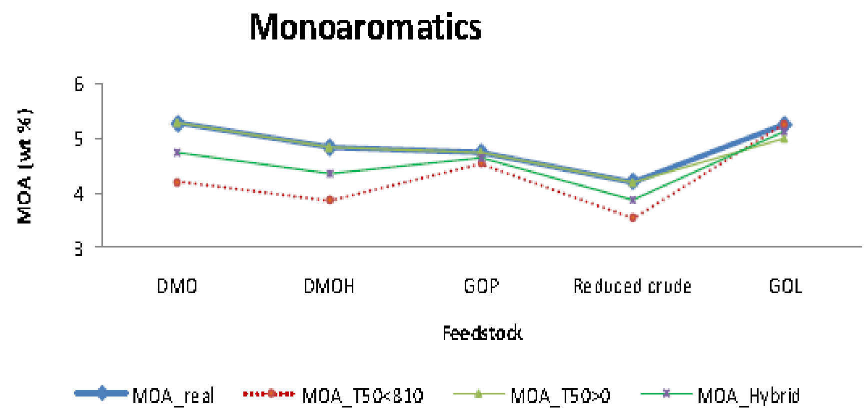
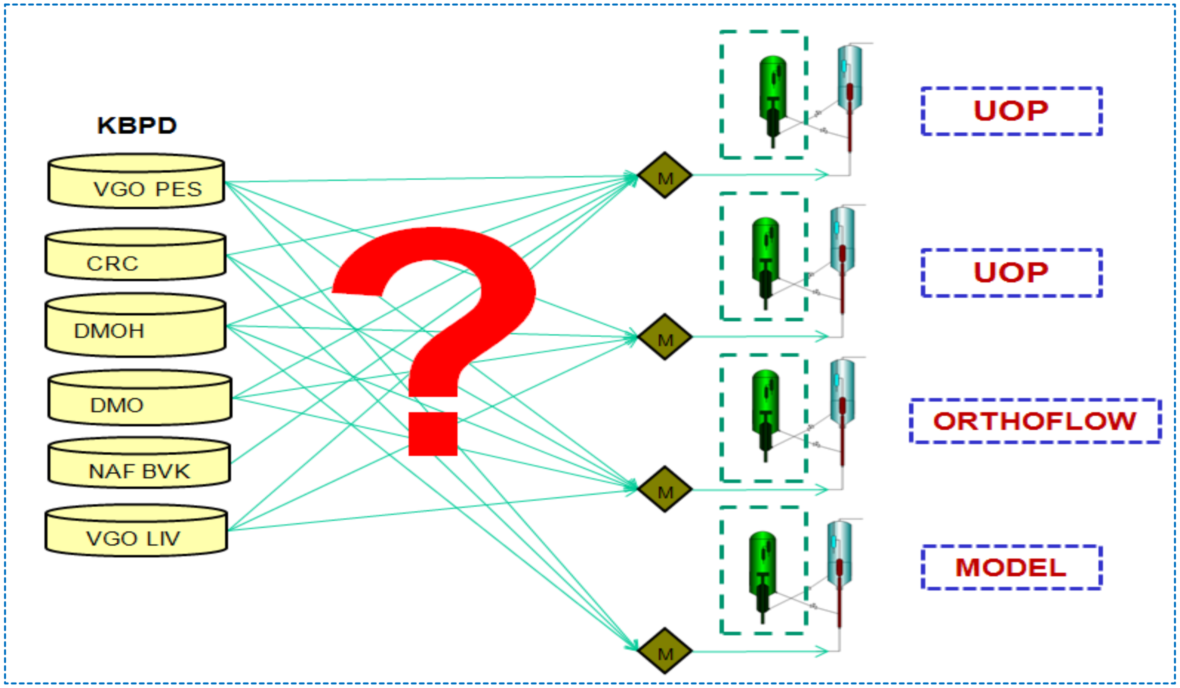


Figure B-6. Correlation for monoaromatics.

The segmented correlations were implemented using continuous variables, resulting in MPCC. This MPCC problem was automatically reformulated (through the penalty reformulation) as an NLP in GAMS using the NLPEC solver

Feedstock Planning for FCC



Optimizing

Feed Allocation

$T_{preheat}$

$T_{reaction}$

Maximizing Yields

or

Profit

Optimal Solution of SIGMA-FCC

	UOP I	UOP II	ORTHO FLOW	MODEL IV
T rxn (°F)	984.32	970.50	975.00	916.00
T preheat ((°F)	350.00	430.00	390.00	350.00
Feed (Kbpd)				
GOP	14.61	28.00	13.64	12.69
DMOH	10.30	3.80	0.00	0.00
DMO	0.00	0.00	5.67	0.00
Reduced crude	0.00	0.00	0.00	0.00
Naphtha	0.09	1.00	0.70	0.81
GOL	0.00	0.00	0.00	0.00
Total	25.0	32.8	20.0	13.5
Nonlinear elements	765	Objective ($)		800 816

Conclusions

- Original FCC model developed in EcoPetrol contains logistic constraints as well as highly nonlinear and segmented empirical correlations. It is difficult to be used in planning tool SIGMA-FCC.
- By introducing MPCC and reformulating the correlations and constraints of FCC, SIGMA-FCC becomes efficient and effective to be used.
- Preliminary results of optimal solutions show potential power of SIGMA-FCC in EcoPetrol
- Currently extended to larger FCC models, integrated with refinery