Feedstock Characterization and Model Reformulation for SIGMA-FCC in EcoPetrol

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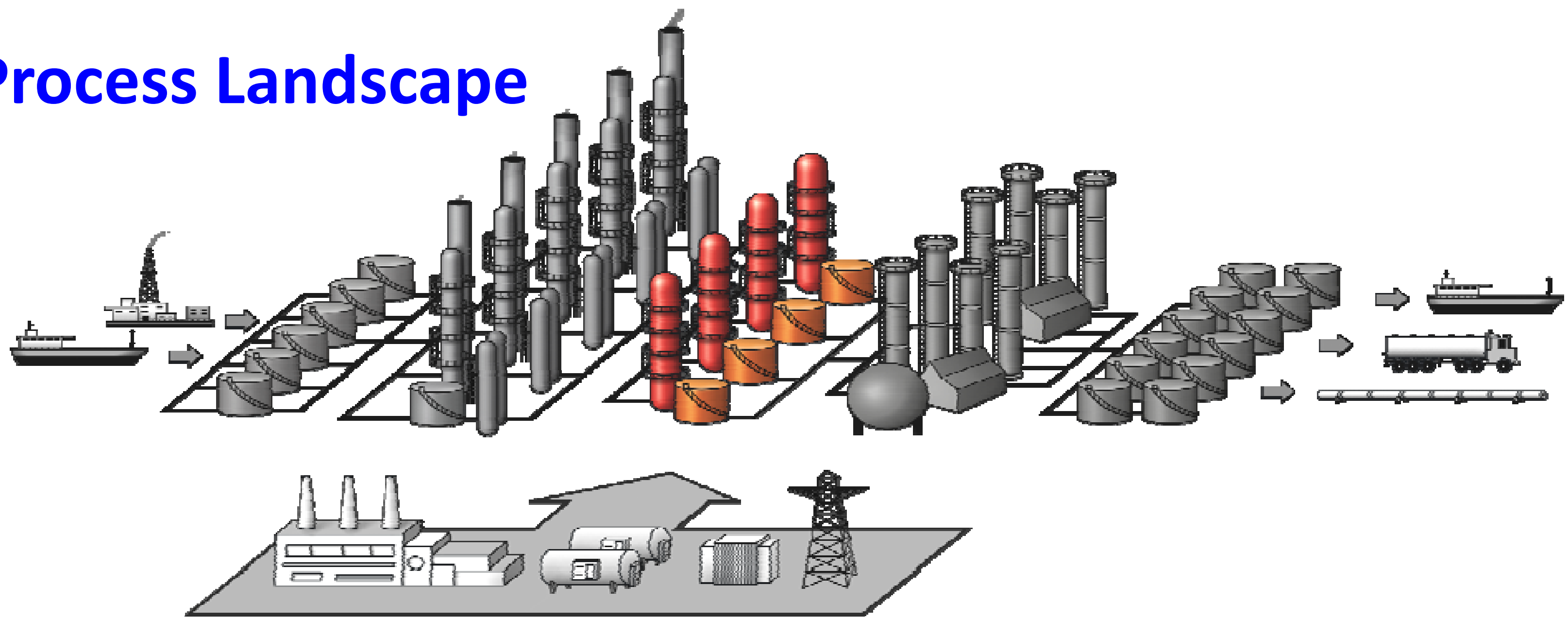
Outlines

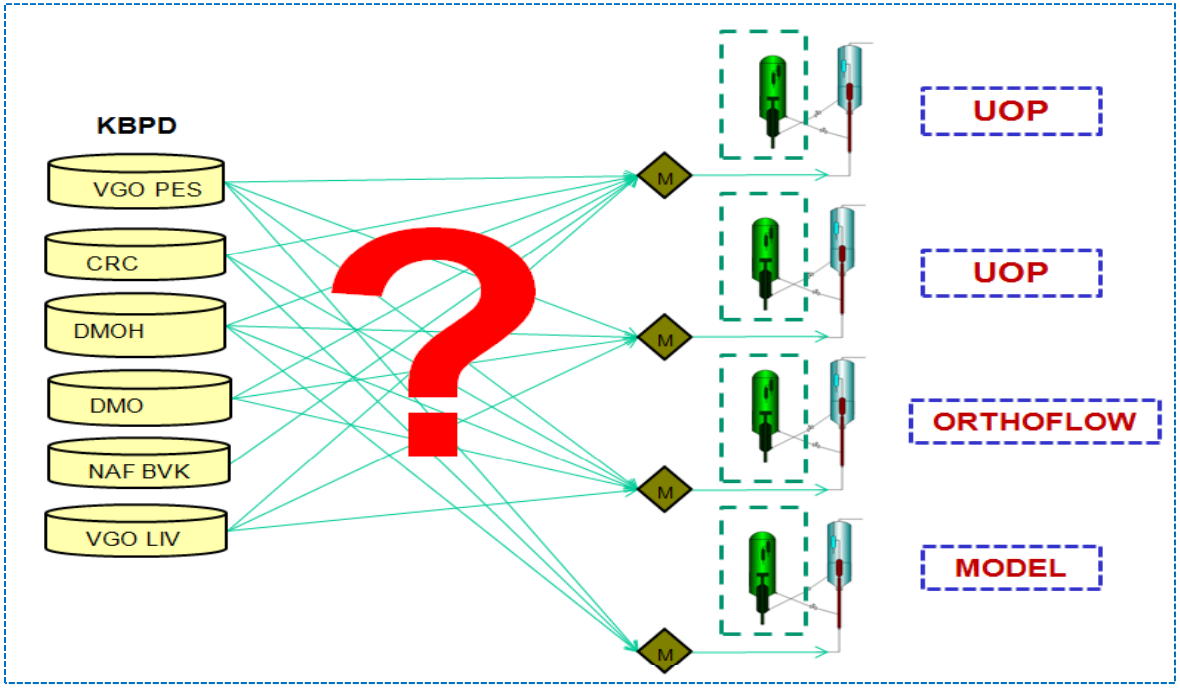
- Introduction
- Challenges
- Project Design
- Activities through EWO
- Progresses stage by stage
- Conclusions

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

Process Landscape



Feedstock Planning for FCC



Optimizing

Feed Allocation

$T_{preheat}$

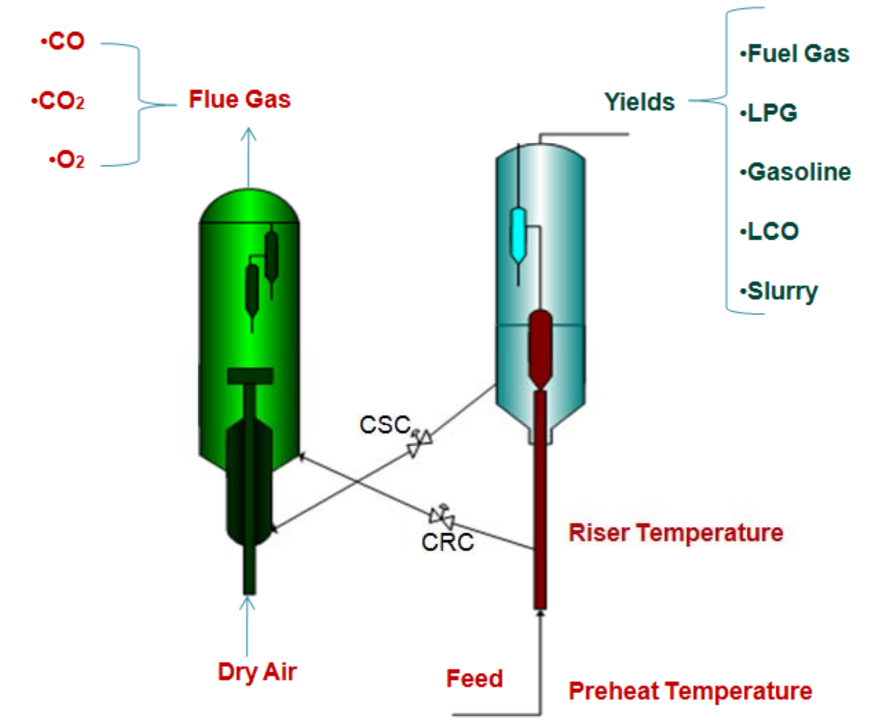
$T_{reaction}$

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

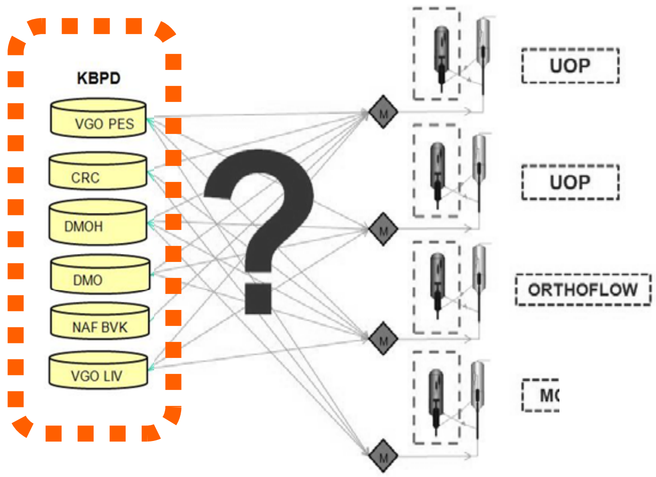
Sulphur Limit
Conradson Carbon Limit

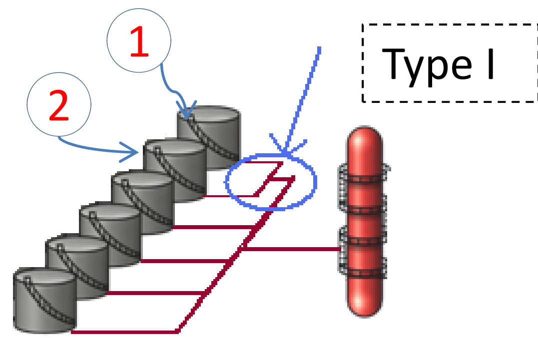
Coke Constraints

Coke Burnt and Produced

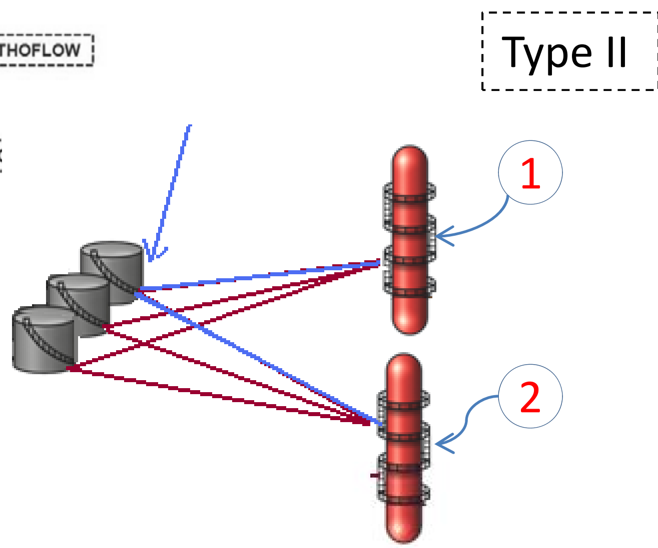
Logistic Constraints

Selecting feedstock for each unit of FCC





$$y_1 + y_2 = 1$$
$$0 \le y_1 \perp y_2 \ge 0$$
$$z = f_1(x)y_1 + f_2(x)y_2$$



$$y_1 + y_2 = 1$$
$$0 \le y_1 \perp y_2 \ge 0$$
$$z_i = f_{i,1}(x)y_1 + f_{i,2}(x)y_2$$
$$i = 1,2,3$$

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

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
417 100000

Project Definition

1. Reformulate models from MINLP into NLP
2. Reformulate models to improve their mathematical properties
3. Introduce new developed technologies to solve NLP with better performances (e.g. Ipopt with PAT)

Challenges

- Models are blind for CMU because they are EcoPetrol proprietary
- High nonlinearity --- Complicated empirical correlations in the models
- Discontinuity --- Segmented correlations in the models
- Complementarity --- Logistic constraints in the models

Outlines of project design

- Reformulate the planning problems as Nonlinear programming (NLP) problems
- Reformulate the models with common techniques such as nonlinear reduction, variable scaling,…
- Reformulated the models with the techniques developed here, e.g. MPCC
- Try to use novel NLP solver such as Ipopt, therefore, for more convenience, translate the models from GAMS into AMPL
- Using parameter adaptive tuning (PAT) for Ipopt to solve the problems

Activities through EWO program

- Preliminary contact, Professors Biegler and Grossmann visit EcoPetrol, give seminars, get basic information and relative materials.
- Kick-off and following discussions in Pittsburgh during 2010 EWO meeting (March). The report 1 from EcoPetrol was presented to CMU, the CMU submitted a set of suggestions to the partner.
- on April 26, 2010, CMU got the Report 2 from EcoPetrol
- On July 26, 2010, CMU got the report 3 from EcoPetrol with a paper outlines led by this project
- On Aug. 12, 2010, CMU sent EcoPetrol the comments and suggestions on the report 3.
- On Sept. 28, 2010, A presentation of the project is given in EWO meeting
- At AIChE 2010 annual meeting, Larry and Ariel have a discussion.
- On Nov. 26, 2010. A report of performances of Ipopt with two Planning models in AMPL is sent to CMU from EcoPetrol.
- CMU solves the two models successfully with Ipopt using PAT (Parameter Adaptive Tunning) technique and the results sent to EcoPetrol.
- On January 14, 2011, CMU got workplan for 2011 from EcoPetrol

Progresses Stage by Stage

When the project started, original comparison among the solver shows (Report #1)

- SBB, DICOPT & CONOPT are almost the same
- MINOS failed for all cases
- SNOPT failed 75%
- KNITRO failed 50%
- IPOPT solved all cases with
  the same solutions for two cases; a little differences for other two

	Case I			Case II			Case III			Case IV		
	Profit (M$US)	CPU (S)	No. iter	Profit (M$US)	CPU (S)	No. iter	Profit (M$US)	CPU (S)	No. iter	Profit (M$US)	CPU (S)	No. iter
SBB	**741.99**	**0.73**	**259**	**749.11**	**0.70**	**252**	**800.85**	**1.09**	**432**	**801.03**	**0.86**	**439**
DICOPT	**741.99**	**0.63**	**259**	**749.11**	**0.51**	?	**800.85**	**2.12**	**1922**	**801.03**	**1.06**	**439**
CONOPT	**741.99**	**0.42**	**208**	**749.11**	**0.48**	?	**800.85**	**0.82**	**270**	**801.03**	**0.76**	**439**
MINOS	---	---	---	---	---	---	---	---	---	---	---	---
SNOPT	---	---	---	**749.11**	**2.95**	**5343**	---	---	---	---	---	---
KNITRO	---	---	---	---	---	---	**800.85**	**1.76**	?0	**801.03**	**8.85**	**?0**
IPOPT	**729.61**	**1.14**	**73**	**749.04**	**2.42**	**129**	**796.42**	**4.34**	**221**	**801.03**	**12.78**	**524**

Suggestions from CMU after diagnosis: Reformulate models, invoke MPCC

Reformulation model

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

Ipopt got improvement after MPCC reformulation

Solver performance for the FCC model reformulation

Solver	*MPCC without reformulation*		*MPCC with reformulation*	
	CPU time (s)	Profit (US$)	CPU time (s)	Profit (US$)
CONOPT	0.321	800.816	0.297	800.816
MINOS	Infeasible	Infeasible	Infeasible	Infeasible
SNOPT	Infeasible	Infeasible	Infeasible	Infeasible
KNITRO	Infeasible	Infeasible	Infeasible	Infeasible
IPOPT	4.731	796.567	1.969	800.816

Results of linearization
for Highly Nonlinear Correlations
(Report #3)

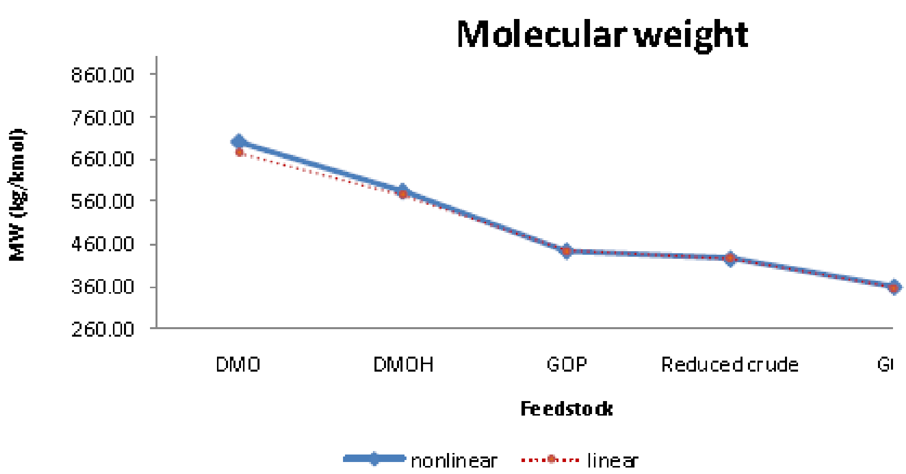


Figure A-1. Correlation for molecular weight.

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

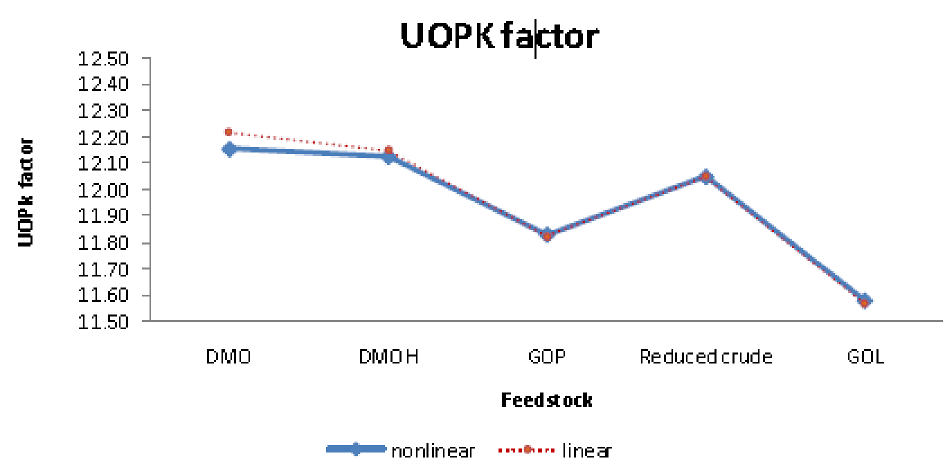


Figure A-2. Correlation for UOPk factor.

Results of smoothing segmented correlations

(Report #3)

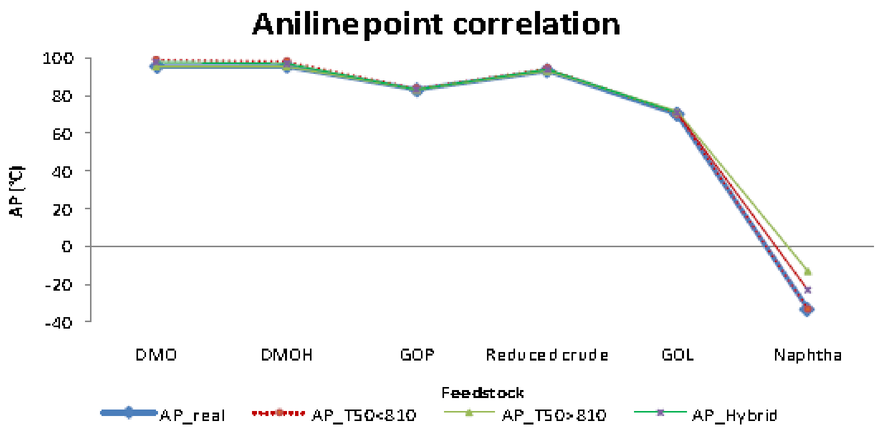


Figure B-1. Correlation for aniline point.

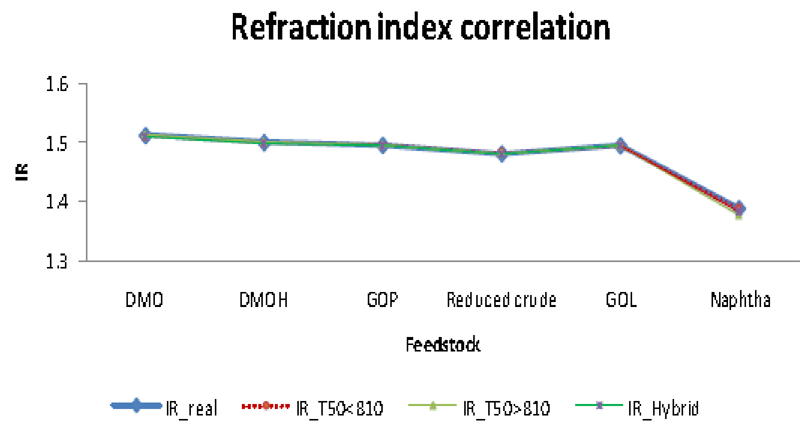


Figure B-2. Correlation for refraction index.

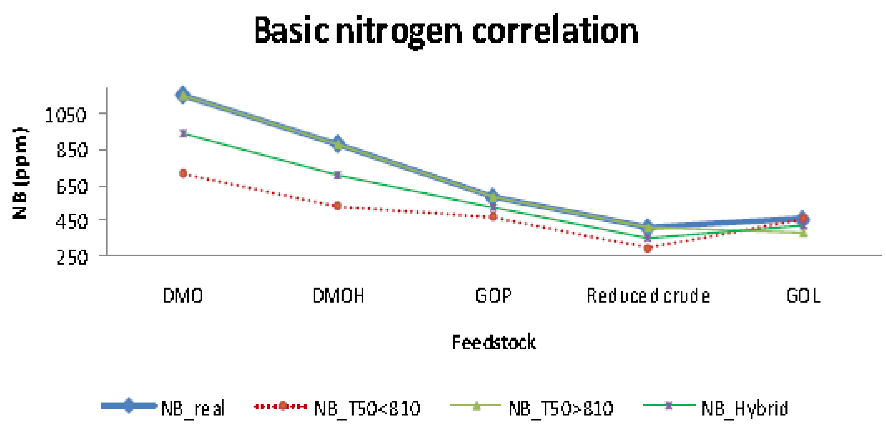


Figure B-3. Correlation for basic nitrogen.

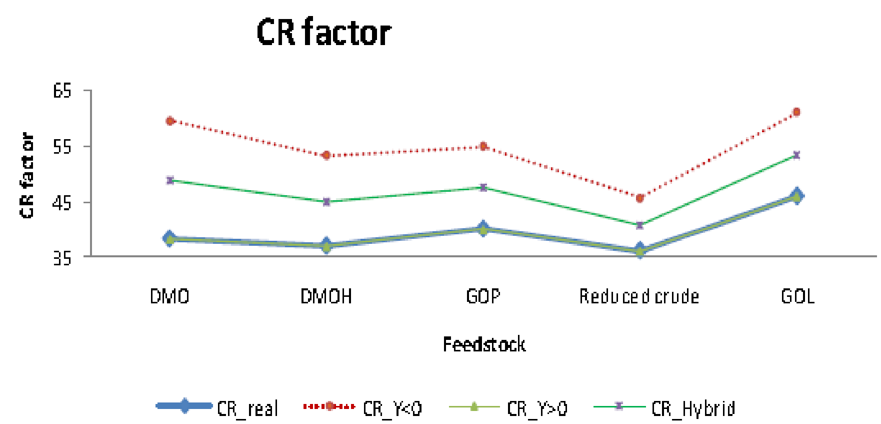


Figure B-4. Correlation for CR factor.

Results of smoothing segmented correlations (Cont'd.)

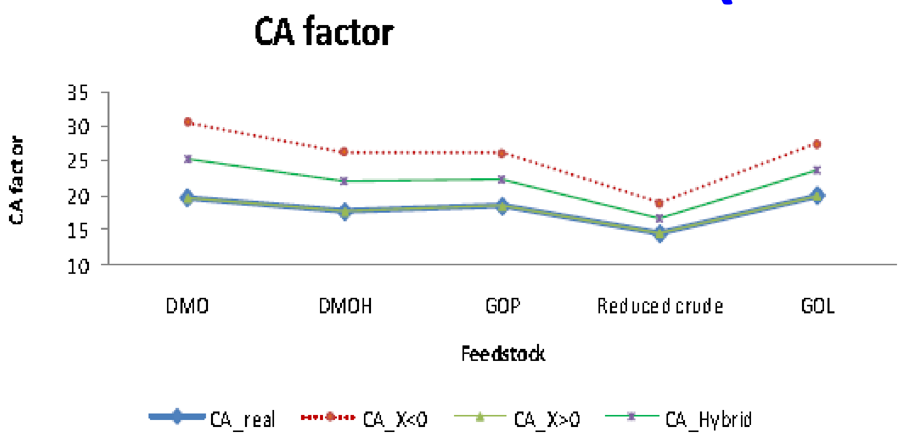


Figure B 5. Correlation for CA factor.

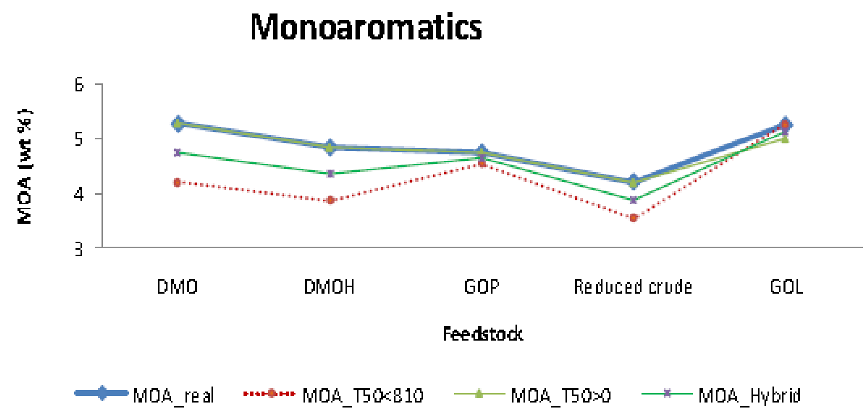


Figure B-6. Correlation for monoaromatics.

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

Mathematical Program with Complementary Constraints
MPCC

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

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

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

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

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 be embedded within a standard Non-Linear Programming solver and obtain fast local solutions
+ Computation generally scales polynomially with problem size
- Introduces an inherent non-convexity and constraint dependency

Ipopt failed to solve two new practical cases

Solver performance (ECOPETROL´s refineries)			
RCSA			
CONOPT		IPOPT	
**** SOLVER STATUS	1 Normal Completion	**** SOLVER STATUS	3 Resource Interrupt
**** MODEL STATUS	2 Locally Optimal	**** MODEL STATUS	6 Intermediate Infeasible
**** OBJECTIVE VALUE	541.9985	**** OBJECTIVE VALUE	0
RESOURCE USAGE, LIMIT	0.109 , 1000.000	RESOURCE USAGE, LIMIT	1000.216, 1000.000
GRB			
CONOPT		IPOPT	
**** SOLVER STATUS	1 Normal Completion	**** SOLVER STATUS	3 Resource Interrupt
**** MODEL STATUS	2 Locally Optimal	**** MODEL STATUS	6 Intermediate Infeasible
**** OBJECTIVE VALUE	1592.2608	**** OBJECTIVE VALUE	0
RESOURCE USAGE, LIMIT	18.081, 1000.000	RESOURCE USAGE, LIMIT	1000.435, 1000.000

Note: Computer Info: Intel(R) Pentium(R) Dual CPU T2390 @ 1.86GHz (CPU:0). 2,00 GB de RAM
GAMS version : 23.5.2
Ipopt version: 3.8stable, running with linear solver mumps

Suggestions from CMU: Introduce PAT for Ipopt

Results of invoking PAT: From failure to success

Solver performance (ECOPETROL´s refineries)		
RCSA		
	Default	**Tuned**
Objective	532.0365	541.9985
Dual infeasibility	1.04E+02	3.15E-08
Constraint violation	2.41E-05	9.09E-13
Complementarity	6.55E-06	1.94E-12
Solver status	Maximum of Iterations Exceeded	Optimal Solution Found
Number of Iterations	3.00E+03	8.80E+01
Total CPU secs	52.84	2.25

Solver performance (ECOPETROL´s refineries)				
GRB				
	Original GRB with Default Parameter Settings	**Scaled GRB with Tuned Parameter Settings**		**Unscaled GRB**
Objective	1003.1108	**1595.7305**		**1595.7305**
Dual infeasibility	1.92E+00	6.21E-07	→	
Constraint violation	1.16E-06	**5.19E-12**		**5.50E-07**
Complementarity	3.86E-05	1.01E-10		
Solver status	Maximum of Iterations Exceeded	Optimal Solution Found		
Number of Iterations	3.00E+03	9.36E+02		
Total CPU secs	969.35	170.14		

Note: Computer Info: Genuine Intel(R) CPU T2300 @ 1.66GHz. 1.5 GB de RAM
GRB is scaled. Ipopt version: 3.8.3, running with linear solver ma27

Performance Comparison of CONOPT with Tuned Ipopt

Solver performance (ECOPETROL´s refineries)			
RCSA			
CONOPT		IPOPT	
**** SOLVER STATUS	1 Normal Completion	**** SOLVER STATUS	Optimal Solution Found
**** MODEL STATUS	2 Locally Optimal	**** MODEL STATUS	
**** OBJECTIVE VALUE	541.9985	**** OBJECTIVE VALUE	541.9985
RESOURCE USAGE, LIMIT	0.109 , 1000.000	RESOURCE USAGE, LIMIT	2.25 1000.000
GRB			
CONOPT		IPOPT	
**** SOLVER STATUS	1 Normal Completion	**** SOLVER STATUS	Optimal Solution Found
**** MODEL STATUS	2 Locally Optimal	**** MODEL STATUS	
**** OBJECTIVE VALUE	1592.2608	**** OBJECTIVE VALUE	**1595.7305**
RESOURCE USAGE, LIMIT	18.081, 1000.000	RESOURCE USAGE, LIMIT	170.14, 1000.000

Note: Computer Info: Intel(R) Pentium(R)
Dual CPU T2390 @ 1.86GHz (CPU:0). 2,00 GB de RAM
GAMS version : 23.5.2
Ipopt version: 3.8stable, running with linear solver mumps

Tuned Parameters by PAT for Ipopt to solve two practical cases

Parameter Setting Proposed by PAT for SP-RCSA

Parameter Name	Parameter Value
alpha_for_y	max
alpha_for_y_tol	1.52E+01
barrier_tol_factor	6.48E+00
bound_frac	2.17E-02
bound_mult_init_method	constant
bound_mult_init_val	1.85E+00
bound_push	1.97E-02
fixed_mu_oracle	loqo
max_soc	0
mu_init	5.55E-02
mu_linear_decrease_factor	3.14E-01
mu_max	9.58E+04
mu_max_fact	1.33E+03
mu_min	5.16E-13
mu_oracle	quality-function
mu_strategy	adaptive
mu_superlinear_decrease_power	1.19E+00
nlp_scaling_max_gradient	9.54E+01
obj_scaling_factor	3.02E-01
quality_function_max_section_steps	3
linear_solver	ma57

Parameter Setting Proposed by PAT for GRB

Parameter Name	Parameter Value
alpha_for_y	min-dual-infeas
alpha_for_y_tol	3.06E+00
barrier_tol_factor	1.22E+01
bound_frac	1.76E-02
bound_mult_init_method	mu-based
bound_mult_init_val	1.28E+00
bound_push	1.85E-02
fixed_mu_oracle	loqo
max_soc	3
mu_init	1.40E-01
mu_linear_decrease_factor	2.65E-01
mu_max	1.32E+05
mu_max_fact	1.80E+03
mu_min	5.62E-13
mu_oracle	quality-function
mu_strategy	adaptive
mu_superlinear_decrease_power	1.38E+00
nlp_scaling_max_gradient	6.38E+01
obj_scaling_factor	1.07E+00
quality_function_max_section_steps	11
linear_solver	ma27
hessian_approximation	limited-memory

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.
- By invoking PAT, Ipopt becomes more robust
- Preliminary results of optimal solutions show potential power of SIGMA-FCC in EcoPetrol
- EWO is still helpful even for handling enterprise proprietary