The Performances Estimation of the FCC Plant Using Numerical Treatment of the Castiglioni Method

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Castiglioni method is a graphical method used to estimate product yield obtained in the catalytic cracking unit. Basically, the graphical methods are difficult to apply and don't allow a direct numerical processing of the input data. The article develops a numerical technique using the Castiglioni method and based on this, it develops a calculus program for predicting the product yield for the catalytic cracking unit. The comparison of the numerical results obtained by applying the calculus algorithm and the example presented by the Castiglioni method allowed the validation of the algorithm. Four study cases of operating the catalytic cracking unit have been analysed using the calculus program.

Keywords: yield prediction, catalytic cracking, numerical methods

One of the most important processing oil units from a refinery is the catalytic cracking unit. This ensures the conversion of the heavy distillates into products with high energy and economic potential, such as gasoline, diesel, and gases et.al. The performances of this process depend on a number of factors such as: the type of feedstock, the degree of conversion, operating temperature et. al. The catalytic cracking process management requires a quick estimation of the yield and quality reaction products. This can be done based on rigorous mathematical models or by using correlation between the yields of the products obtained, the feedstock properties and the operating conditions.

Over the years in the technical literature various correlations for predicting the yields of the products obtained in the catalytic cracking process have been published. Gay and Handwerk suggest a correlation between conversion and specific gravity [1]. Castiglioni and Jones published different graphic correlations between product yields and feedstock properties (the volumetric average boiling point, specific gravity, aniline point, sulphur content) [2, 3]. Maples presents a correlation between product yields and the characterization factor of the feedstock, the conversion, the sulphur content in feedstock and the gravity of the feedstock. He compares his correlations with Baker's [5], Gary's [1] and Nelson's [6], demonstrating that his correlations are better. Al-Enzi et al. presents the prediction of the yields based on an approximation function using the regression algorithm type [7]. More recent preoccupations are presented in the related published papers [8-10].

Because the Castiglioni method is a graphical method which involves a heavy use, the authors have studied and elaborated a numerical treatment of this method. The calculus program realised based on numerical treatment can be quickly used to predict the yield and the quality of the reaction products.

Numerical treatment of castiglioni method

The Castiglioni method is applicable to catalytic cracking units that produce gasoline with a final temperature of 204 °C and which are operated with a catalyst containing 0.2% carbon mass on the regenerated catalyst, the feedstock properties having the values presented in table 1 [2].

Table 1
THE FEEDSTOCK PROPERTIES

Properties	Units measure	Values
Volumetric average boiling point	°C	443
Specific density d_{15}^{15}	-	0.910
Aniline Point	°C	92
Sulphur	% masa	0.5
The feedstock conversion	% vol	85
The feedstock flow	kg/h	225000

Starting from the original Castiglioni method, the authors have developed a numerical algorithm, algorithm which reflects the step calculations presented in the original article [2].

Calculation of the corelation factor

The correlation factor of the feedstock, α, is defined through the relation (1)

$$\alpha = 75 - 0.065\,T_{mbp} - 0.9\,S + 0.6\,P_a - 0.26\,\frac{P_a}{\rho_{feed}} \quad (1)$$

Yield of the C_3 - 204°C *hydrocarbon fraction*

The yield of the C_3 - 204°C *hydrocarbon fraction* can be predicted through a bi-dimensional quadratic interpolation of the discrete function presented in the graphical algorithm, figure 1 from article [2]

$$C_{3-204} = g_1(Conv, \alpha). \quad (2)$$

Gasoline yield

The ratio between the yield of the C_5 - 204°C hydrocarbon fraction and the yield of the C_3 - 204°C hydrocarbon fraction can be estimated based on the next relation

$$\frac{C_{5-204}}{C_{3-204}} = f_1(\alpha) = -5.2777772134\times10^{-7}\alpha^3 + 4.1309511896\times10^{-5}\alpha^2 + 1.5626976138\times10^{-3}\alpha + 8.3180950693\times10^{-1}. \quad (3)$$

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The gasoline yield, respectively C_5 - 204°C fraction, can be calculated based on the following relation

$$C_{5-204} = \frac{C_{5-204}}{C_{3-204}} C_{3-204} \cdot \quad (4)$$

Yield of C_3 and C_4 hydrocarbon fraction

The yield of the $C_3 + C_4$ hydrocarbon fraction is obtained from the difference between C_3 - 204°C fraction and C_5 - 204°C fraction

$$C_3 + C_4 = C_{3-204} - C_{5-204}. \quad (5)$$

The ratio between the C_4 hydrocarbon fraction and the C_3 hydrocarbon yield can be estimated based on the function (6), determined by polynomial regression

$$\left(\frac{C_4}{C_3}\right) = f_2(\alpha) = -8.055556963\text{E}\times10^{-7}\alpha^3 + 1.1702381273\times10^{-4}\alpha^2 - 9.556349439\times10^{-3}\alpha + 2.1458333386. \quad (6)$$

The yield of the C_3 hydrocarbon fraction is calculated based on the relation

$$C_3 = \frac{C_3 + C_4}{1 + \frac{C_4}{C_3}} \cdot \quad (7)$$

The yield of the C_4 hydrocarbon fraction is obtained from the difference between the yield of the (C_3 + C_4) hydrocarbon fraction and the yield of the C_3 hydrocarbon fraction

$$C_4 = (C_3 + C_4) - C_3. \quad (8)$$

Propylene yield

The ratio of the propylene yield and C_3 hydrocarbon yield can be predicted with the approximation function

$$\left(\frac{C_{propylene}}{C_3}\right) = f_3(\alpha) = 5.965226691\times10^{-1} + 1.3016997165\times10^{-3}\alpha. \quad (9)$$

The propylene yield is calculated with the following relation

$$C_{propylene} = \left(\frac{C_{propylene}}{C_3}\right) C_3. \quad (10)$$

The rest of the hydrocarbons from the C_3 fraction can be predicted based on the difference between the C_3 hydrocarbon yield and propylene yield

$$C_{3rest} = C_3 - C_{propylene}. \quad (11)$$

Butylene yield

The ratio between the butylene yield and the C_4 hydrocarbon fraction yield can be estimated based on the approximation function

$$\left(\frac{C_{butylene}}{C_4}\right) = f_4(\alpha) = 3.6013968254\times10^{-1} + 1.775555536\times10^{-3}\alpha. \quad (12)$$

The butylene fraction yield is calculated with the following relation

$$C_{butylene} = \left(\frac{C_{butylene}}{C_4}\right) C_4. \quad (13)$$

The rest of the C_4 hydrocarbon fraction can be calculated as the difference between the yield of C_4 hydrocarbon obtained in step 8 and the yield of the butylene fraction

$$C_{4rest} = C_4 - C_{butylene}. \quad (14)$$

The yield of the n-butane fraction is calculated based on the relation

$$C_{n-butane} = 0.125\, C_4. \quad (15)$$

The yield of the i-butane fraction is calculated based on the difference between the yield of the rest of C_4 hydrocarbon fraction and the yield of the n-butane fraction

$$C_{i-butylene} = C_{4rest} - C_{n-butane}. \quad (16)$$

Yield of the coke, C_2 fraction and lighter gases

The yield of the coke, C_2 fraction and lighter gases is estimated using the bi-dimensional quadratic interpolation of the discrete function from the graphical algorithm

$$(C_{coke} + C_{2\&LG}) = g_2(Conv, \alpha). \quad (17)$$

The ratio between the coke yield and the yield of the mixture between coke, C_2 fraction and lighter gases is determined by the bi-dimensional quadric interpolation of the discrete function presented in figure 7 in article [2]

$$\left(\frac{C_{coke}}{C_{coke} + C_{2\&LG}}\right) = g_3(Conv, \alpha). \quad (18)$$

The coke yield is calculated with the following relation

$$C_{coke} = \left(\frac{C_{coke}}{C_{coke} + C_{2\&LG}}\right) \times (C_{coke} + C_{2\&LG}). \quad (19)$$

The yield of the C_2 fraction and the lighter gases is determined based on the relation

$$C_{2\&LG} = (C_{coke} + C_{2\&LG}) - C_{coke}. \quad (20)$$

The estimation of the C_2 and the lighter gases yield is achieved assuming the distribution of these components according to table 2 and then recalculating the composition based on the relation

$$C_i = \frac{C_i \times C_{2\&LG}}{100}, \quad i = 1,\ldots,4. \quad (21)$$

Table 2
THE CONCENTRATION OF C_2 COMPONENT AND LIGHTER GASES

No	Component	The approximate composition [% masă]
1	Hydrogen	1.7
2	Methane	41.3
3	Ethylene	23.0
4	Ethane	34.0
Total		100.0

Yield of the sulphide hydrogen

In order to calculate the H_2S yield, firstly we must determine the H_2S ratio on the sulphur from the feedstock

using the approximation function

$$\left(\frac{C_{H2S}}{Feed}\right) = f_5(\alpha) = 1.5217586936\times10^{-5}\alpha^2 - 7.2060177270\times10^{-3}\alpha + 8.3424941196\times10^{-1}, \quad (22)$$

The yield of the sulphide hydrogen is calculated based on the relation

$$C_{H2S} = \left(\frac{C_{H2S}}{Feed}\right)\times S. \quad (23)$$

Gasoline yield

The density of the gasoline containing hydrocarbons starting from the C_5 fraction to the final temperature 204°C hydrocarbons, density which expressed in °API, is determined through the bi-dimensional quadratic interpolation of the discrete function shown in figure 9 in article [2]

$$d_{API\_gas} = g_4(Conv, \alpha). \quad (24)$$

The relative density of the gasoline is calculate based on the relation

$$d_{15\_gas} = \frac{141.5}{131.5 + d_{API\_gas}}. \quad (25)$$

The gasoline yield of the catalytic cracking unit will be

$$C_{gas} = C_{5-204}\frac{d_{15\_gas}}{\rho_{feed}}. \quad (26)$$

Oil yield

The oil yield is defined as the difference between 100% volume (feed in) and the conversion of the feedstock

$$C_{CO\_vol} = 100 - Conv. \quad (27)$$

The passage from the yield expressed in % volume to the yield expressed in % mass is achieved through bidimensional quadric interpolation of the discrete function presented in figure 10 in article [2].

$$\left(C_{CO\_mass} - C_{cycleoil\_vol}\right) = g_5(Conv, \alpha). \quad (28)$$

The mass yield of the oil is

$$C_{CO\_mass} = \left(C_{CO\_mass} - C_{CO\_vol}\right) + C_{CO\_vol}. \quad (29)$$

Assuming that the heavy oil is 5 % volume from the oil yield, the light oil yield is

$$C_{LCO\_vol} = C_{CO\_vol} - 5. \quad (30)$$

There are three steps to be followed in order to calculate the mass yield of the light oil. Initially a correction factor is determined, through a bidimensional quadric interpolation of the discrete function presented in figure 11 of the article [2]

$$FF = g_6(Conv, \alpha). \quad (31)$$

The feedstock density, expressed in °API, is given by

$$d_{feed\_API} = \frac{141.5}{\rho_{feed} - 131.5} \quad (32)$$

and light oil density will be

$$d_{LCO\_API} = \rho_{feed} - FF. \quad (33)$$

The passage to the relative density, corresponding to the 15°C temperature is

$$d_{LCO} = \frac{141.5}{131.5 + d_{LCO\_API}}. \quad (34)$$

The mass yield of the light oil is defined as

$$C_{LCO\_mass} = C_{LCO\_vol}\frac{d_{LCO\_mass}}{\rho_{feed}}. \quad (35)$$

The mass yield of the heavy oil is the difference between total mass yield of the oil and the mass yield of the light oil

$$C_{DO\_mass} = C_{CO\_mass} - C_{LCO\_mass} \quad (36)$$

and density of the heavy oil fraction will be

$$d_{DOs} = \rho_{feed}\frac{C_{DO\_mass}}{C_{DO\_vol}}. \quad (37)$$

Estimation of the gasoline octane number

The motor octane number is estimated through the bidemensional quadratic interpolation of discrete function presented in figure 12 of the article [2]

$$COM = g_7(Conv, \alpha). \quad (38)$$

and the research octane number is estimated through the bi-dimensional quadratic interpolation of the discrete function presented in figure 12 of the article [2]

$$COR = g_8(Conv, \alpha). \quad (39)$$

The calculation program

The calculation program has a sequential structure. The approximation functions $f_1,\ldots, f_5$ have been determined through polynomial regression and are implemented through type function modules presented in [11]. The functions $g_1,\ldots, g_8$ are approximation functions which utilise the bi-dimensional interpolation algorithms. The calculation program generates an output file that contains both the partial and the final results of the numerical calculation.

Study cases

The estimation program of the catalytic cracking unit performance has been tested utilising the primary data presented in the afore mentioned article [2]. In table 3 presents comparatively the original results of the Castiglioni method and the ones obtained by applying the numerical algorithm developed by the authors. The average quadratic error of the numerical algorithm is 0.24% mass, value which validates the numerical algorithm elaborated by the authors.

The numerical algorithm has been utilised for the estimation of a Romanian catalytic cracking unit performance. The primary data from table 4 contains four operating data.

In table 5 presents the results obtained by applying the numerical algorithm for the four cases studies, in comparison with the industrially obtained data. The errors between the two categories of results are synthetically depicted in table 6.

Component	Castiglioni article		Numeric algorithm	
	calculated	normalized	calculated	normalized
Hydrogen	0.05	0.05	0.05	0.06
Methane	1.21	1.23	1.31	1.40
Ethylene	0.67	0.68	0.73	0.78
Ethane	0.99	1.00	1.08	1.15
Propylene	4.50	4.57	3.97	4.26
Propane	1.83	1.86	1.62	1.73
Butylene	6.28	6.37	6.72	7.21
Izo-butylene	4.31	4.37	5.59	5.99
n-Butane	1.51	1.53	1.34	1.43
Gasoline	52.07	52.84	46.82	50.18
Lighter oil	13.45	13.45	12.11	12.98
Heavy oil	5.70	5.70	5.16	5.53
Coke	6.08	6.08	6.53	7.00
Hydrogen sulphide	0.27	0.27	0.27	0.29
Total	98.92	100.00	93.3	99.99

Table 3
COMPARATIVE VALUES OF THE COMPONENTS [% MASS]

Properties	Measurement units	Case 1	Case 2	Case 3	Case 4
Volumetric average boiling point	°C	390	414	380	404
Specific density at 15°C	-	0.9200	0.9383	0.9000	0.9050
Aniline point	°C	75.6	75.6	79.4	83.3
Sulphur	% mass	0.35	1.55	0.18	0.40
Conversion of the feedstock	% vol	75	70	82	85
The feedstock flow	kg/h	188600	125000	150000	175000

Table 4
OPERATING DATE FROM CATALYTIC CRACKING UNIT

Table 5
COMPARISON BETWEEN PRODUCTS YIELD OBTAINED IN FCC UNIT [% MASS]

Component	Case 1		Case 2		Case 3		Case 4	
	Model	Industrial	Model	Industrial	Model	Industrial	Model	Industrial
Hydrogen	0.05		0.04		0.06		0.07	
Methane	1.14		0.95		1.42		1.61	
Ethylene	0.64		0.53		0.79		0.9	
Ethane	0.94		0.78		1.17		1.32	
Propylene	3.67		3.2		4.21		4.23	
Propane	1.52		1.35		1.72		1.73	
Butylene	6.41		5.76		7.16		7.23	
Izo-butylene	5.21		4.57		5.93		5.97	
n-Butane	1.26		1.11		1.42		1.43	
Total Gases	**20.84**	**21.7**	**18.29**	**19.6**	**23.88**	**23.6**	**24.49**	**24.7**
Gasoline	**47.31**	**48.5**	**44.93**	**45.2**	**50.36**	**51.6**	**51.45**	**52.5**
Lighter oil	19.99		24.9		13.01		10.13	
Heavy oil	5.56		5.66		5.56		5.69	
Total oil	**25.55**	**25.3**	**30.56**	**30**	**18.57**	**19.2**	**15.82**	**17.1**
Coke	**6.18**	**5.5**	**5.61**	**5.2**	**7.14**	**5.6**	**8.09**	**5.7**
Hydrogen sulphide	0.13		0.60		0.07		0.15	

Table 6
ERROR BETWEEN CALCULATE AND INDUSTRIAL DATA

Component	Error [% mass]
Gases	0.64
Gasoline	1.03
Oil	0.60
Coke	2.17
Average	1.11

The smallest error is registered for oil, 0.60%, while the biggest error is registered for coke, respectively 2.17%. Overall the numerical algorithm elaborated based on the Castiglione method registers an average error of 1.11%, fact which validates with industrial data this algorithm.

Conclusions

The current paper renders a synthetic presentation of the authors' research results regarding the development of a calculus program designed to estimate the product yield of the catalytic cracking. The calculus program is based on one of the numerical treatment methods known in the specialised literature as the Castiglioni method. The article introduces the calculus stages which lay at basis of numerical methods of estimating product yield. The comparative analysis of the numerical results obtained through the proposed calculus algorithm and the example presented by the Castiglioni methods has confirmed the effectiveness of the studies algorithm. The case studies, based on industrial data, validate the numerical algorithm developed by authors.

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Nomenclature

T_{mbp} - Volumetric average boiling point
ρ_{feed} - Gravity d_{15}^{15} of the feedstock
P_a - Aniline point

S - Sulphur
$Conv$ - Conversion of the feedstock
Q_{feed} - Feedstock flow
α - Correlation factor
$C_{3\text{-}204}$ - The yield fraction that contain hydrocarbons from C_3 to hydrocarbons with final 204°C
$C_{5\text{-}204}$ - The yield fraction that contain hydrocarbons from C_5 to hydrocarbons with final 204°C
C_3+C_4 - C_3+C_4 fraction yield
C_3 - C_3 hydrocarbon yield
C_4 - C_4 hydrocarbon yield
$C_{propylene}$ - Propylene fraction yield
C_{3rest} - C_3 hydrocarbon fraction yield without propylene
C_4 - C_4 hydrocarbon fraction yield
$C_{butylene}$ - Butylene fraction yield
C_{4rest} - C_4 hydrocarbon fraction yield without butylenes
$C_{n\text{-}butane}$ - n-butane hydrocarbon fraction yield
$C_{i\text{-}butylene}$ - i-butylene hydrocarbon fraction yield
C_{coke} - Coke yield
$C_{coke}+C_{2\&LG}$ - Coke, C_2 and lighter gases yield
$C_{2\&LG}$ - C_2 hydrocarbon and lighter gases yield
C_{H2S} - Hydrogen sulphide
d_{API_gas} - Density gasoline expressed in şAPI (hydrocarbons from C_5 to hydrocarbon whit finale temperature 240°C)
C_{CO_vol} - Oil yield, % volume
C_{CO_mass} - Oil yield , % mass
C_{LCO_vol} - Lighter oil yield , % volume
d_{LCO} - Gravity of the lighter oil

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