# FCC-DD A SOFTWARE APPROACH OF THE CASTIGLIONI METHOD FOR FCC YIELDS PREDICTION

**Raluca-Elena Dragomir** [1]

**Bogdan Doicin** [1]

[1] Petroleum-Gas University of Ploiesti, **Romania**
e-mail: ralued@yahoo.co.uk

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## ABSTRACT

This paper presents an improved method of determining the products yields obtained in the Fluid Catalytic Cracking (FCC) process based on the Castiglioni graphical method, using FCC-DD v1.0 a program written in the Python programming language. The advantage of using FCC-DD is the speed and accuracy of the obtained results, as well as avoidance reading of the diagrams, these being discretized and incorporated into the software.

**Keywords:** Python, FCC DD, Castiglioni method, yields

## INTRODUCTION

Since 1942 when the first commercial FCC was introduced, it has been one of the most important conversion technologies in the oil processing industry.

Intended for the manufacture of gasoline as the main product, the catalytic cracking process was first carried out in a fixed-bed reactors, followed shortly by fluidized bed reactors.

Using of a zeolite catalyst in the catalytic cracking process led to the significant evolution of the quality of the obtained products. Gasoline with a high octane number, more stable gases and residues in smaller quantities are obtained, this being achieved at conversions of over 90%. [1]

The FCC process converts heavy feedstocks such as gas oil, heavy crude oil and residues into products with high economic value and a high quality. It is one of the cheapest processes which converting heavy oil fractions into high octane gasoline, propylene and gases for the petrochemical industry. [2, 3]

Currently, over 350 FCC plants are operating worldwide with a total processing capacity of over 12.7 million barrels/day.

The flexibility of the process can help the refinery in changing the product mix, given the current decline in the quality of feedstocks.

Although it has been used for many years, FCC remains the process with the largest weight in the processing of crude oil and continues to develop both through the improvement of the catalysts used and through the current trend of using other raw materials. [4, 5]

Due to the depletion of oil resources, the increasing $CO_2$ emissions and global warming phenomena the trend is to use feedstocks obtained from biomass or biomass mixed with petroleum fractions in the presence of the cracking catalysts. [6]

The present work propose the predict of products yields obtained in the FCC process, using the FCC-DD v1.0 software wrote in PYTHON language, based on the method proposed by Castiglioni.

**Presentation of the Castiglioni Method**

The estimation of the yield of products was made for a feedstock with characteristics similar to those used in the industrial FCC plant currently. The method uses the type of feedstock, the level of conversion and the degree of catalyst activity. The conversion level and activity of the catalyst are chosen.

To determine the yield of the reaction products and their properties, the Castiglioni graphical method correlates the conversion, with a correlation factor "α", which synthetically expresses the quality of the raw material, characterized by: volumetric average boiling point (VABP), aniline point (AP), specific gravity (SG), sulfur content [wt %]. The calculations are done in stages following a 24 steps sequence. [7]

**Presentation of the FCC-DD Created Software**

For the software approach of the Castiglioni method, FCC-DD program was conceived. This software computes the FCC Yields according to the Castiglioni method. FCC-DD v1.0 was wrote using the Python programming language, version 3.9.10 and the PyCharm Community Edition, IDE, version 2021.3.2. Both the programming language and the IDE are free and can be downloaded from their web pages. [8, 9]

The main advantage of the FCC-DD is the speed of computing. Without the aid of a computer, the calculations needed a large amount of time to be completed. By using the developed program, the results are computed and displayed in a few seconds.

Another very important advantage is that all the nomograms and the diagrams used in the 24 steps of the method are discretized and embedded into the software. All values that had to be read from graphs and nomograms are now calculated by interpolation. It has been observed that small differences occur between the interpolated values and those read by a human directly from the graphs. The difference is given by the interpolation results, which depend on the number of points read from the graphs. If this number is larger, the interpolation will be more accurate, leading to negligible errors.

To be able to compute the FCC yields, according to the Castiglioni method, FCC-DD needs the following input data:

- Feed flow (tons per year);
- Conversion level (% vol.);
- Temperatures at 10%, 50% and 90% on the ASTM curve (°C);
- Specific gravity;
- Sulfur content (wt. %).

Those inputs are read from a text file, which must be in the order specified above.

After the calculation, the results are displayed in a tabular format and in a text file as well.

To implement the Castiglioni method, the authors divided the program into the following modules:

- Main – it is responsible with running the computations engine and saving the results into the text file;
- Conversions – responsible for different conversions between units of measure;
- Engine – the module that performs the computations of the Castiglioni method;
- Print to file – responsible with arranging the results into a tabular shape and saving everything into a results file;
- Steps – this module contains the mathematical representations of the 24 steps of the Castiglioni method. The Engine module uses them and makes them work together. Without this module, these steps are independent one of another;
- Backend – this module is responsible of all the computations from the backend, all the computations used in the other modules, except for the Main module.

## RESULTS AND DISCUSSIONS

To prove that the developed FCC-DD program is accurate, it was tested on a set of inputs, which are presented in Table 1:

*Table 1* Feed properties

| **Property (UOM)** | **Value** |
|---|---|
| Feed flow (t/yr.) | 1600000 |
| Conversion level (% vol.) | 75 |
| Temperature at 10% on the ASTM curve(°C) | 315 |
| Temperature at 50% on the ASTM curve(°C) | 430 |
| Temperature at 90% on the ASTM curve(°C) | 530 |
| Specific gravity | 0.905 |
| Sulfur content (% wt.) | 0.45 |

The Castiglioni method was used, with the inputs given in Table 1 to determine the FCC yields. It was used both manually (Castiglioni) and by using the FCC-DD. The obtained results are presented comparatively as following.

*Table 2* Comparative results for steps 1 to14 obtained manually and by using software FCC-DD

| **Property (UOM)** | **Value** | |
|---|---|---|
| | Manually | FCC-DD |
| Aniline point (°F) | 180 | 180 |
| Correlation factor | 79.077 | 79.08 |
| **Property (UOM)** | **Value** | |
| | Manually | FCC-DD |
| Yield of $C_3$ – 400°F fraction (% vol.) | 80.6 | 80.61 |
| **Property (UOM)** | **Value** | |
| | Manually | FCC-DD |
| $C_5$ – 400°F/ $C_3$ – 400°F ratio | 0.7 | 0.7 |
| **Property (UOM)** | **Value** | |
| | Manually | FCC-DD |
| Yield of $C_5$ – 400°F (% vol.) | 56.72 | 56.72 |
| **Property (UOM)** | **Value** | |
| | Manually | FCC-DD |
| Yield of $C_3$ + $C_4$ fraction (% vol.) | 23.88 | 23.88 |
| **Property (UOM)** | **Value** | |
| | Manually | FCC-DD |
| Total $C_4$ ratio to total $C_3$ ratio | 1.68 | 1.68 |
| **Property (UOM)** | **Value** | |
| | Manually | FCC-DD |
| Yield of total $C_3$ (% vol) | 8.9 | 8.9 |
| **Property (UOM)** | **Value** | |
| | Manually | FCC-DD |
| Yield of total $C_4$ (% vol) | 14.98 | 14.98 |
| **Property (UOM)** | **Value** | |
| | Manually | FCC-DD |
| Propene yield (% vol) | 6.3 | 6.3 |
| $C_3$ Remainder (% vol.) | 2.61 | 2.61 |
| **Property (UOM)** | **Value** | |
| | Manually | FCC-DD |
| Butene yield (% vol.) | 7.59 | 7.59 |
| Butane yield (% vol.) | 1.87 | 1.87 |
| Isobutane yield (% vol.) | 5.52 | 5.52 |

| Property (UOM) | Value | |
|---|---|---|
| | Manually | FCC-DD |
| Yield of coke, $C_2$ and lighter (% vol.) | 7.3 | 7.29 |
| **Property (UOM)** | **Value** | |
| | Manually | FCC-DD |
| Coke ratio to the total of the coke + $C_2$ and lighter | 0.675 | 0.68 |
| **Property (UOM)** | **Value** | |
| | Manually | FCC-DD |
| Yield of coke (% wt.) | 4.93 | 4.93 |
| **Property (UOM)** | **Value** | |
| | Manually | FCC-DD |
| Yield of $C_2$ and lighter (% wt.) | 2.37 | 2.36 |

The results for step 15 are presented in Table 3 and Table 4. Table 3 represents the manually obtained results and Table 4 represents the results obtained by the software program. Table 5 represents the difference and the error.

*Table 3* Results for step 15, obtained manually

| Component | Based on avg., % wt. | Based on fresh feed, % wt. |
|---|---|---|
| Hydrogen | 1.7 | 0.04 |
| Methane | 41.3 | 0.97 |
| Ethene | 23 | 0.54 |
| Ethane | 24 | 0.80 |
| Total | 100 | 2.37 |

*Table 4* Results for step 15, obtained by using the FCC-DD software

| Component | Based on avg., % wt. | Based on fresh feed, % wt. |
|---|---|---|
| Hydrogen | 1.7 | 0.04 |
| Methane | 41.3 | 0.97 |
| Ethene | 23 | 0.53 |
| Ethane | 24 | 0.80 |
| Total | 100 | 2.36 |

*Table 5* The difference and error between the two methods

| **Component** | **Difference** | | **Error (%)** | |
|---|---|---|---|---|
| | Based on avg | Based on fresh feed | Based on avg | Based on fresh feed |
| Hydrogen | 0 | 0 | 0 | 0 |
| Methane | 0 | 0 | 0 | 0 |
| Ethene | 0 | 0,01 | 0 | 0.04 |
| Ethane | 0 | 0 | 0 | 0 |

*Table 6* Comparative results for steps 16 to 21 obtained manually and by using software FCC-DD

| **Property (UOM)** | **Value** | |
|---|---|---|
| | Manually | FCC-DD |
| Hydrogen sulfide yield (% wt.) | 0.171 | 0.17 |
| **Property (UOM)** | **Value** | |
| | Manually | FCC-DD |
| Gasoline yield (% wt.) | 46.84 | 46.84 |
| **Property (UOM)** | **Value** | |
| | Manually | FCC-DD |
| Yield of total cycle oil (% wt.) | 26.1 | 26.16 |
| **Property (UOM)** | **Value** | |
| | Manually | FCC-DD |
| Light cycle oil (% vol.) | 20 | 20 |
| **Property (UOM)** | **Value** | |
| | Manually | FCC-DD |
| Light cycle oil (% wt.) | 20.53 | 20.41 |
| **Property (UOM)** | **Value** | |
| | Manually | FCC-DD |
| Decant oil gravity | 1.00 | 1.04 |

The results for step 22 are presented in Table 7 and Table 8. Table 7 represents the results obtained manually and Table 8 represents the results obtained by FCC-DD software program.

*Table 7* The results from step 22 obtained by the manual method

| Component | Vol % | SG | Yield (%) | |
|---|---|---|---|---|
| | | | Calculated | Normalized |
| Hydrogen | - | - | 0.04 | 0.04 |
| Methane | - | - | 0.97 | 1.06 |
| Ethene | - | - | 0.54 | 0.59 |
| Ethane | - | - | 0.80 | 0.87 |
| Propene | 7.02 | 0.52 | 4.05 | 4.41 |
| Propane | 2.90 | 0.50 | 1.62 | 1.77 |
| Butene | 8.45 | 0.60 | 5.61 | 6.11 |
| Isobutene | 6.13 | 0.56 | 3.81 | 4.15 |
| n-butane | 2.08 | 0.58 | 1.34 | 1.46 |
| $C_5$ – 400°F | 54.00 | 0.74 | 44.34 | 48.29 |
| Light cycle oil | 20 | 0.92 | 20.53 | 20.53 |
| Decant oil | 5 | 1.00 | 5.56 | 5.56 |
| Coke | - | - | 4.92 | 4.92 |
| Hydrogen sulfide | - | - | 0.17 | 0.1 |
| Total | 105.60 | 0.90 | 94.37 | 100.00 |

*Table 8* The results from step 22 obtained by FCC-DD software program

| Component | Vol % | SG | Yield (%) | |
|---|---|---|---|---|
| | | | Calculated | Normalized |
| Hydrogen | 0 | 0 | 0.04 | 0.04 |
| Methane | 0 | 0 | 0.97 | 1.03 |
| Ethene | 0 | 0 | 0.54 | 0.58 |
| Ethane | 0 | 0 | 0.8 | 0.85 |
| Propene | 6.30 | 0.52 | 3.29 | 3.50 |
| Propane | 2.61 | 0.51 | 1.32 | 1.41 |
| Butene | 7.59 | 0.6 | 4.56 | 4.86 |
| Isobutene | 5.52 | 0.56 | 3.11 | 3.31 |
| n-butane | 1.87 | 0.58 | 1.09 | 1.17 |
| $C_5$ – 400°F | 56.72 | 0.74 | 46.84 | 49.92 |

| | | | | |
|---|---|---|---|---|
| Light cycle oil | 20 | 0.93 | 20.41 | 21.75 |
| Decant oil | 5 | 1.03 | 5.75 | 6.13 |
| Coke | 0 | 0 | 4.93 | 5.26 |
| Hydrogen sulfide | 0 | 0 | 0.17 | 0.18 |
| Total | 105.61 | 0.79 | 93.82 | 100 |

The results for step 23 are presented in Table 7 and in Table 8. Table 7 presents the results obtained by the manual method and Table 8 presents the results obtained by FCC-DD.

*Table 7* The results from step 23 obtained by the manual method

| **Component** | **Yield** | | **Sulfur** | | | |
|---|---|---|---|---|---|---|
| | | | Calc (step 23) | | Normalized | |
| | Wt.% | Lb./h | Wt.% | Lb./h | Wt.% | Lb./h |
| Gasoline | 48.29 | 96587.18 | 0.1 | 96.59 | 0.05 | 54.11 |
| Light cycle oil | 20.54 | 41077.15 | 1 | 410.77 | 0.56 | 230.15 |
| Decant oil | 5.56 | 11122.85 | 2.5 | 278.07 | 1.40 | 155.80 |
| Coke | 4.93 | 9855.00 | 2.5 | 246.38 | 1.40 | 138.04 |
| Total above | 79.32 | 158642.18 | 0 | 1031.80 | 0 | 578.11 |
| Sulfur in $H_2S$ | 0 | 0 | 0 | 0 | 0 | 321.88 |
| Total sulfur | 0 | 0 | 0 | 0 | 0 | 900 |

*Table 8* The results from step 23 obtained by the FCC-DD software program

| **Component** | **Yield** | | **Sulfur** | | | |
|---|---|---|---|---|---|---|
| | | | Calc (step 23) | | Normalized | |
| | Wt.% | Lb./h | Wt.% | Lb./h | Wt.% | Lb./h |
| Gasoline | 46.84 | 94055.83 | 0.1 | 94.06 | 0.06 | 52.62 |
| Light cycle oil | 20.41 | 40894.62 | 1 | 409.85 | 0.56 | 229.27 |
| Decant oil | 5.75 | 11.540.65 | 2.5 | 288.52 | 1.40 | 161.40 |
| Coke | 4.93 | 9904.48 | 2.5 | 247.61 | 1.40 | 138.52 |
| Total above | 77.92 | 156845.58 | 0 | 1040.03 | 0 | 581.80 |
| Sulfur in $H_2S$ | 0 | 0 | 0 | 0 | 0 | 321.89 |
| Total sulfur | 0 | 0 | 0 | 0 | 0 | 903.69 |

The results for step 24 are presented in Table 9.

*Table 9* Comparative results for step 24 obtained manually and by using software FCC-DD

| **Property (UOM)** | **Value** | |
|---|---|---|
| | Manually | FCC-DD |
| MON | 80 | 80.96 |
| RON | 91.2 | 91.8 |

## CONCLUSIONS

The FCC process has revolutionized the refining industry, being the most widespread conversion process applied worldwide. The developed FCC-DD result in quickly and accurately tool for estimating of the reaction product yields using the Castiglioni method.

The difference between the manual method and the FCC-DD software program depends only on the interpolation data.

The developed "FCC-DD v1.0" will be improved and made "user friendly". For the future versions authors intend to improve the graphical user interface and make the program to be able to read inputs in different measuring units and also to generate the results from results file in other units of measure as well.

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