

# Modelling the Atmospheric Distillation Using the Unisim Design Simulator

*Cristian Patrascioiu*<sup>1\*</sup>

<sup>1</sup>Automatic Control, Computers & Electronics Department, Petroleum-Gas University of Ploiesti, Romania

**Abstract.** The process of atmospheric distillation represents the first oil processing process realized in refineries, with a particular impact, both in terms of production and energy. The modeling and simulation of the atmospheric distillation process is one of the tools used to reduce operating costs and increase the efficiency of the industrial plant. The paper aims at presenting research concerning the calculation of liquid-vapor equilibrium for petroleum products as well as an exhaustive analysis of an oil distillation column modeling. The paper is an indispensable didactic component in the mathematical modeling activity of the atmospheric distillation process.

## 1 Introduction

The simulation of the crude distillation process is a challenge in the field of chemical process simulation due to the chemical character of the crude oil subjected to the processing and the complexity of the distillation column. The use of chemical process simulators is the current method used to simulate the crude distillation process. The thermodynamic model selection is the first issue to be addressed in simulating the atmospheric distillation process.

The author suggests a review of the paper [1], which analyses Peng-Robinson and Chao-Sea thermodynamic models. The authors of the article recommend using the Aspen Hysys Assistant - Property Method Selection (APMS) module to select the most appropriate thermodynamic model. In paper [8] it is mentioned the use of a model of the stationary regime of the crude distillation column, which is realised in the HYSYS simulation environment. The paper presents results obtained in the dynamical simulation of a quality control system based on DMC simulation, the two simulators communicating through specific channels. A handbook about designing a simulator for atmospheric distillation column is presented in paper [2] in which the simulation environment is Aspen HYSYS. Although the user interface and the commands used are specific to this simulation environment, the user can exploit its concepts and adapt them to her own simulation environment. The simulator HYSYS v8.6, a version closer to the Unisim Design simulator, used to simulate a crude distillation column is presented in paper [3]. The defining elements of the paper are: the exhaustive treatment of light components, water and hydrocarbon

---

\*

Corresponding author: [cpatrascioiu@upg-ploiesti.ro](mailto:cpatrascioiu@upg-ploiesti.ro)

pseudo components; preheating the feed stream; shaping the atmospheric distillation column as a reflux absorption column; pump-around implementation; selecting the specifications used to solve the mathematical model.

Other references about the use of Aspen HYSYS and HYSYS simulators are published in [5-7].

Literature also refers to the use of the PRO II simulator for modelling and simulating an crude distillation column [4]. The cited academic handbook is intended for the design and economic analysis of all equipment used in the atmospheric distillation plant.

In this context, the author has initiated researches in the field of modelling and simulation of the atmospheric distillation process, the most recent achievements being presented in the paper [9].

## 2 Calculation of liquid-vapor equilibrium for petroleum products

The liquid-vapor equilibrium was studied for a Romanian crude oil from the Băicoi reservoir, characterized by the PRF curve [10]. Based on these experimental data, the author has approached two methods for calculating liquid-vapor balance for crude oil and petroleum products derived from it as well as for other physical properties. The two methods are: the method based on the Edmister-Okamoto correlations [11] and the method based on the transformation of the petroleum product into a mixture of pseudo-constituents [12].

### 2.1 Method based on Edmister-Okamoto correlations

Basically, petroleum products are characterized by:

- the real PRF boiling point curve used as the reference curve in the product characterization;
- vaporization curve in VE equilibrium, used for calculations associated with liquid-vapor equilibrium;
- STAS distillation curve, used for a fast characterization of the product.

Edmister-Okamoto correlations are experimentally determined functions that correlate the real boiling point curve TBP, the equilibrium vapor curve FVE and the ASTM distillation curve of the crude oil and petroleum products. The method based on the Edmister-Okamoto correlations calculates the potential of white products (gasoline, petroleum, diesel oil) and the main temperatures in the CDU column. Based on this methodology, the author has developed a complex program that treats the liquid-vapor equilibrium associated with crude oil and petroleum products separated in a crude distillation column.

The input data of the calculation program are: the TBP curve of the crude oil; the final temperature imposed on the ASTM curve of each distilled fraction and the temperature gap on the ASTM curve imposed between two adjacent fractions, table 1.

**Table 1.** Quality specifications for petroleum products resulting from crude oil processing.

| Fraction name | Final ASTM temperature [°C] | Gap ASTM temperature [°C] |
|---------------|-----------------------------|---------------------------|
| Naphta        | 140                         | 15                        |
| Gasoline      | 205                         | 25                        |
| Petroleum     | 270                         | 5                         |
| Diesel        | 330                         | 0.01                      |

The calculation elements of the mathematical model are as follows:

- a) Calculation of product specifications on the TBP curve;
- b) Calculation of white products potential;
- c) Calculation of physical properties curves for crude oil (average percentage curve - density and efficiency curve - density);
- d) Calculation of average properties of distilled fractions (density, molecular weight, characterization factor);
- e) Calculation of the fractions distillation curves (TBP, ASTM, FVE).

More details on the calculation algorithm are presented in paper [11].

The running of the calculation program has generated results, the most important in the context of the present study being the volumetric and molar distribution of the four products separated in the atmospheric distillation column, table 2. It should be noted that the feed of the column is 3.5 million tons per year, which equates to 430000 kg/h flow rate. These results represent the starting point for modelling the crude distillation process.

**Table 2.** Distribution of petroleum products resulting from crude oil processing.

| Distilled Fraction | Distilled volume [%] | Flow rate [m <sup>3</sup> /h] | Flow rate [kmol/h] |
|--------------------|----------------------|-------------------------------|--------------------|
| Naphta             | 11.2                 | 57.77                         | 425.59             |
| Gasoline           | 16.0                 | 82.53                         | 475.19             |
| Petroleum          | 15.8                 | 81.50                         | 260.73             |
| Diesel oil         | 16.5                 | 85.00                         | 372.96             |

## 2.2 Method based on transformation of the petroleum blend into pseudo-chemical components

Chemical process simulators treat petroleum products as pseudo-component blends. To define pseudo-components associated with crude oil, the following steps are required [12]:

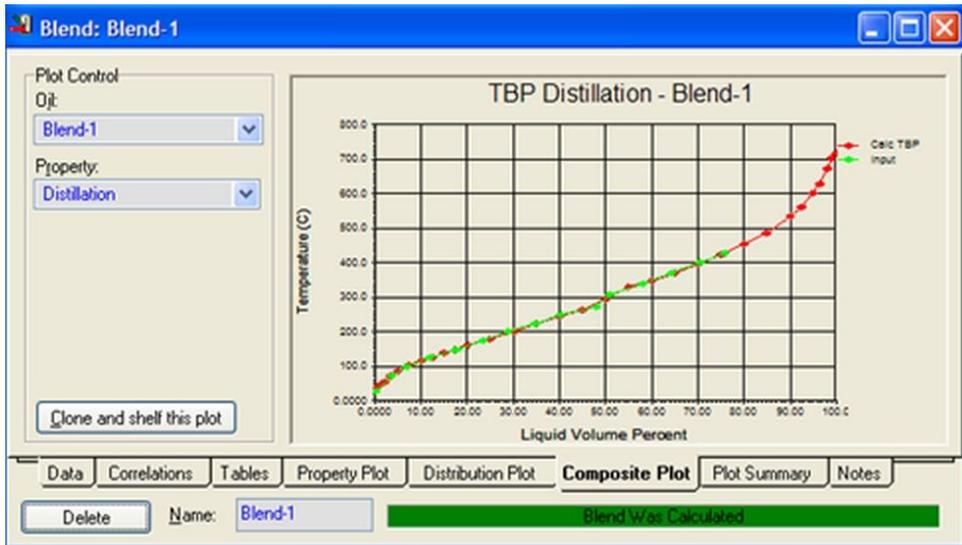
- a) Select the thermodynamic model;
- b) Load of the TBP curve of the petroleum product;
- c) Specification of the petroleum product density curve;
- d) Selection of pseudo-components and calculation of their concentration.

For the thermodynamic model recommended for Peng - Robinson petroleum products, the **Enter Oil Environment** command must be activated to specify the characteristics determined by laboratory analysis. The types of laboratory assays used are listed below: Assay Data Type = TBP; Density Curve = Independent; Input Data = Distillation; Assay Basis = Liquid volume. The values associated with the TBP curve and the values associated with the crude oil density curve. To define the pseudo-components that characterize the crude oil, the **Cut Ranges** function with the **Auto Cut** option is used. After these operations, the crude oil is decomposed into a mixture of pseudo-components.

The calculation of the concentration of each pseudo-component is achieved by minimizing a square function that reflects the deviation between the experimental data and the mixture properties which are calculated based on the pseudo-component properties and their concentration. User validation of the crude oil decomposition is performed by comparing the experimental TBP curve with the TBP curve calculated based on the pseudo-components determined by the simulation program, Figure 1.

The transition to liquid-vapor equilibrium simulation involves loading the list of chemical components with pseudo-components defined within the crude oil, operation triggered by the **Install Oil** control group. The material flow that will use these pseudo-components will be specified in the **Stream Name** or **Feed** window. With this operation,

the definition of the feed flow is completed, next switching to the construction of the mathematical model designed to simulate the atmospheric distillation process.



**Fig. 1.** Comparison of the PRF curve calculated based on the pseudo-components and the experimental curve.

### 3 Modelling the atmospheric distillation process

After the crude oil was assimilated to a mixture of pseudo-constituents and the liquid-vapor equilibrium modelling, the **Feed** stream was obtained. The configuration of this flow is done as it follows:

- The flow temperature is 340 °C, the common temperature in the crude distillation plant;
- The pressure when entering the crude distillation column 2 bar;
- Mass flow rate 430 t/h;
- Volume flow rate 515.6 m<sup>3</sup>/h.

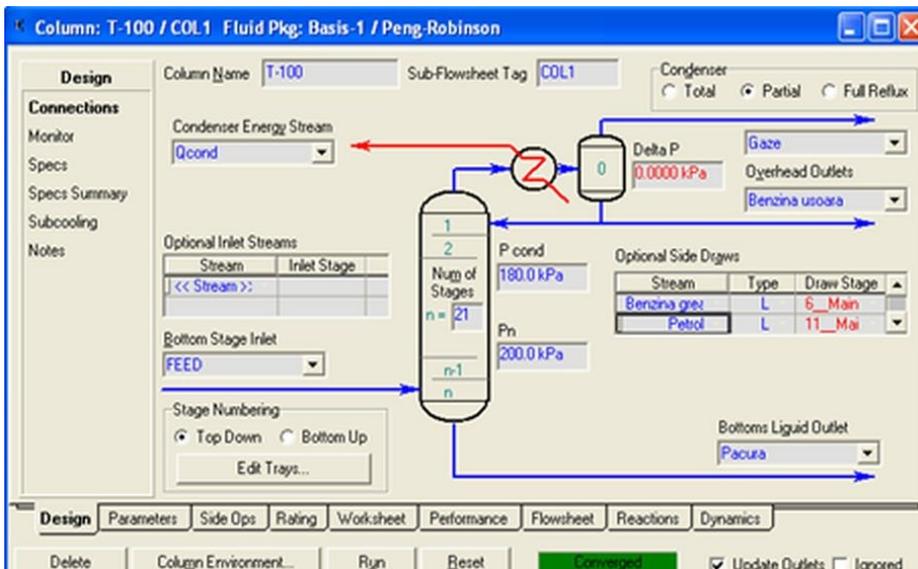
After the crude oil is assimilated to a mixture of pseudo-constituents and the **Feed** flow is obtained, the **Refluxed Absorber** model is imported from the simulator object palette, the configuration of the module being the following:

- a) Feeding the column with **Feed** flow is performed on the tray 21;
- b) Configure the condenser for partial condensation;
- c) Define the gaseous flow in the condenser as **Gaze (Gases)**;
- d) Define the distilled flow as **Benzina usoara (Light gasoline)**;
- e) Define the flow as **Benzina grea (Heavy gasoline)** and position it on the tray 6;
- f) Define the flow as **Petrol (Petroleum)** and position it on the tray 11;
- g) Define the flow as **Motorină (Gasoline)** and position it on the tray 17;
- h) Define the flow from the base column as **Pacura (Naphtha)**;
- i) Define the thermic flow associated with the thermal load of the reboiler as **Qcond**.

After this step, there are configured the following:

- Column profile pressure (1,8 bar at the top, 2 bar at the base);
- Temperature profile within the column (50°C in separator, 120°C at the top, 340°C at the base).

- Estimated molar flow rate for non-condensable flow (19 kmol/h), distillate (425.6 kmol/h), reflux rate (1).
- All these configuration elements are shown in Figure 2.



**Fig. 2.** The configuration elements of the *Refluxed Absorber* module.

At the end of the four configuration steps, the mathematical model cannot be solved, and another mathematical model configuration is required, which involves setting values associated with certain variables of the absorption process. Given the specificity of automatic systems for chemical processes, it is recommended that these variables be the control agents associated with the process. Figure 3 shows the classic automation of the atmospheric distillation column. Basically, the specified fixed-value variables must be associated with flows that are used as control agents in automatic control systems. The non-condensing gas absorption column has a total of 6 flows leaving the column, namely: For an absorption column with this flow distribution, the degree of freedom is 5, respectively 5 values of the column-associated flows must be established.

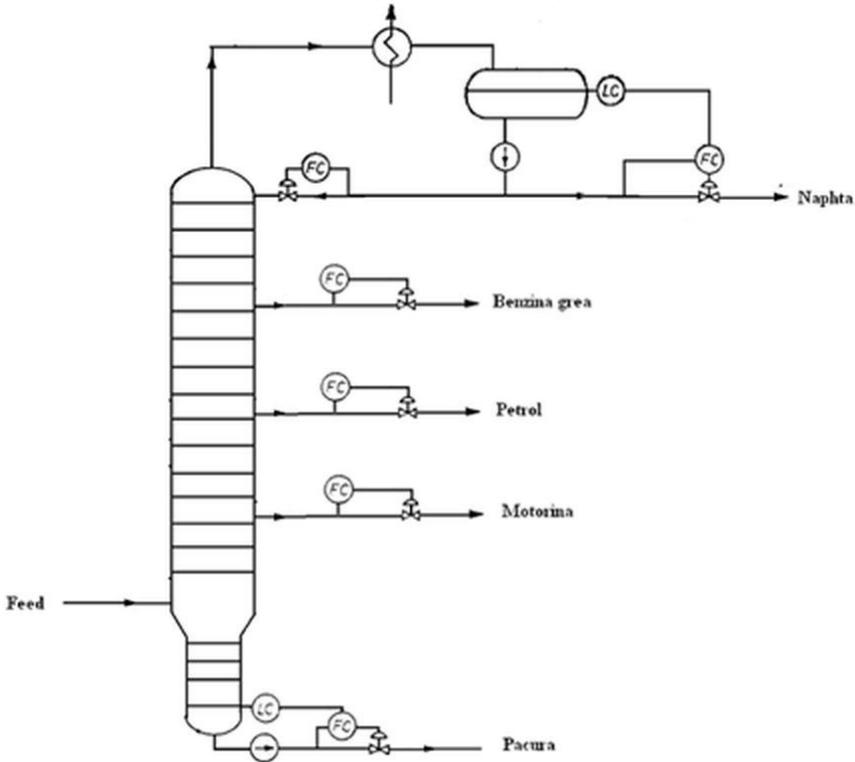
The starting point in the selection of variables is given by the structure of the control system associated with the column. According to it, five independent flow rate control systems are available, namely non-condensable gases, base product, three side fractions and reflux. The variant using the reflux flow rate is not convergent, because in this case there would be two mass flows, the distillate and the base product, which are not defined and implicitly the material balance cannot be closed. In this case, the non-condensable gas variables, the distilled product and the three side fractions were selected, Figure 4.

A sensitive issue is generated by the measurement units of the variables selected as specifications. Considering that these variables will be used within the control systems, the measurement units of these variables will have to be identical to those of these automatic systems, i.e.  $\text{m}^3/\text{h}$  for the flow rate of liquid flows.

The visualization of the distillation curves of petroleum products involves the following steps:

- 1) The absorption column module is selected. The function *Performance* is selected from the available command categories. It calculates the molar flow rate for each pseudo-component existing in petroleum products.

- 2) To view the distillation curves of a petroleum product, the **Plots** option is used. This function calculates the temperatures associated with the distillation curves.
- 3) From the **Assay Curves** command group, the **Boiling Point Assay** and the **View Graph** function are successively selected. In Figure 4, there are exemplified the TBP and ASTM curves of the distilled portion from the processed crude oil.



**Fig. 3.** Classic control structure of the atmospheric distillation column.

|                   | Specified Value | Active                              | Current                             | Fixed/Ranged | Prim/Alt | Lower   | Upper   |
|-------------------|-----------------|-------------------------------------|-------------------------------------|--------------|----------|---------|---------|
| Reflux Ratio      | 1.000           | <input type="checkbox"/>            | <input type="checkbox"/>            | Fixed        | Primary  | <empty> | <empty> |
| Distillate Rate   | 65.00           | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> | Fixed        | Primary  | <empty> | <empty> |
| Reflux Rate       | 300.0           | <input type="checkbox"/>            | <input type="checkbox"/>            | Fixed        | Primary  | <empty> | <empty> |
| Vap Prod Rate     | 19.00           | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> | Fixed        | Primary  | <empty> | <empty> |
| Btms Prod Rate    | <empty>         | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> | Fixed        | Primary  | <empty> | <empty> |
| Benzina grea Rate | 73.00           | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> | Fixed        | Primary  | <empty> | <empty> |
| Petrol Rate       | 81.00           | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> | Fixed        | Primary  | <empty> | <empty> |
| Motorina Rate     | 22.00           | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> | Fixed        | Primary  | <empty> | <empty> |

**Fig. 4.** Summary of specifications used in the distillation absorption column.

The quality control of these products is usually accomplished by adjusting the initial temperature (5% distilled volume) or final (95% distilled volume) of the petroleum product,

temperatures associated with the ASTM curve. The technique described above only allows the visualization of the distillation curves. In order to import these values of the temperature characteristic of the petroleum products, it is necessary to go through other stages. The following is an example of defining a variable containing the temperature value of the ASTM distillation curve for 95% distilled.

- a) The **Tools** menu and the function **Utilities** are chosen from the top bar of the simulator.
- b) To define the variable type, the **UniSim Design Utilities** option is selected and successively the **Available Utilities** command group, the **Boiling Point Curves** function, and the **Add Utility** command.
- c) To define the position of the tray for which the temperature is to be imported, select from within the function **Boiling Point Curves – Connections**, and from **the Object Type** the object **Condenser**, with the **Select Object** button, then select **Condenser**, the independent variable **Basis = Liquid Volume** and **Phase = Liquid**.
- d) Defining the variable to be used in the simulation program involves the use of the **Spreadsheet**. From the **Spreadsheet** Command Bars, choose **Connections**, followed by **Add Import** function. This allows the addition of new simulation program variables. For this purpose, in the **Select Import for Cell** group, select the **Utility** option, the **Boiling Point Curves** object, and in the **Variable** field **the ASTM D86 option, Variable Specifics = Cut Pt-95.00%**.
- e) After defining the Cut Pt-95.00% variable, the program control returns to the **Spreadsheet** mode. The imported variable was stored in cell A1 and its value is available for further processing.
- f) To display the value of the variable stored in cell A1, select the **Spreadsheet** icon, activate the right mouse button and open the **Show Table** function.

Using the procedure described before, the distilled product’s quality values are obtained, and they are presented in Figure 5.

| SPRDSHT-1                    |       |   |
|------------------------------|-------|---|
| A1: ASTM D86 (Cut Pt-95.00%) | 136.2 | C |
| A2: ASTM D86 (Cut Pt-95.00%) | 202.8 | C |
| A3: ASTM D86 (Cut Pt-95.00%) | 263.3 | C |
| A4: ASTM D86 (Cut Pt-95.00%) | 327.9 | C |

**Fig. 5.** The ASTM product qualities.

## 4 Simulation of the atmospheric distillation process

Without industrial data, the starting point of simulations of the atmospheric distillation process is represented by the distribution of products calculated with the Edmister-Okamoto model, according to the imposed quality requirements, Table 1. Using the calculated flow rate with the Edmister-Okamoto model, the Unisim Design simulator will generate a set of temperature associated with the product quality, with temperature sensitively different from those required by the specifications. In this situation, to obtain the same quality of the products as the one imposed, it is necessary to change the product flow rate. Table 3 shows the required value of the final temperature on the ASTM curve compared to the calculated

value of the temperature at 95% distilled on the ASTM curve using the Unisim Design simulator.

Analysis of these values indicates a good and very good correlation for all distilled products. It should be noted that the results presented in Table 3 were obtained after successive attempts, modifying the flow rate of each distilled product according to the following order: naphtha, gasoline, oil and diesel, until the quality condition of each product was met. The deviations expressed in flow rate of the output/used in calculation product are small and medium, except for the diesel product, for which the Edmister-Okamoto model generates substantial errors.

**Table 3.** Comparison between the quality products calculated with the Edmister-Okamoto (EO) method and the Unisim Design (UD) simulator.

| Distilled Fraction | ASTM temperature [°C]     |                                     | Products flow rate [m <sup>3</sup> /h] |                      |
|--------------------|---------------------------|-------------------------------------|--|----------------------|
|                    | Imposed at 100% distilled | Calculated with UD at 95% distilled | Calculated with EO model               | Imposed simulator UD |
| Naphtha            | 140                       | 136.2                               | 57.7                                   | 65                   |
| Gasoline           | 205                       | 202.8                               | 82.5                                   | 73                   |
| Petroleum          | 270                       | 263.3                               | 81.5                                   | 81                   |
| Diesel fuel        | 330                       | 327.9                               | 85.0                                   | 22                   |

## 5 Conclusion

The modelling elements of the atmospheric distillation process were presented in the paper. The fluid-vapor balance of crude oil was treated with the Edmister-Okamoto method and the decomposition method in pseudo-components. The first method was used to estimate the flow rates of products obtained from crude oil distillation, depending on the quality specifications imposed on the products. The second method of calculating liquid-vapor equilibrium is integrated into the Unisim Design simulator, a program simulating the atmospheric distillation column. One of the objectives of the research was the elaboration of the procedure for the calculation and monitoring the properties of the distilled products, using as an example the temperature of the product on the ASTM curve at 95% distilled.

The most important conclusion resulting from the research is the use of the Edmister-Okamoto method only for the rough estimation of the product flow rates in the atmospheric distillation process.

## References

1. J. P. Gutierrez, L.A. Benitez, J. Martinez, L.A. Ruiz, E. Erdmann, *International Journal of Engineering Research and Applications*, **4**, 4 (2014)
2. <http://solutions.aspentech.com/en/aspens-hysys/-/media/self> (accessed 23.03.2019)
3. [http://inside.mines.edu/~jjechura/Refining/Crude\\_Tower\\_Simulation-HYSYS\\_v8.6.pdf](http://inside.mines.edu/~jjechura/Refining/Crude_Tower_Simulation-HYSYS_v8.6.pdf) (accessed 23.03.2019)
4. M. Pearson, V. Vazquez, M. Shum, E. Rademacher, *Crude Distillation Unit - Chemical Engineering Design Project* (University of California, Irvine, 2015)
5. D. D. Gonçalves, F. G. Martins, S. Fayo de Azevedo, *Proceedings of the 20th European Symposium on Computer Aided Process Engineering*, 2010
6. [http://inside.mines.edu/~jjechura/Refining/AspenPlusPetroleumV7\\_1-Start.pdf](http://inside.mines.edu/~jjechura/Refining/AspenPlusPetroleumV7_1-Start.pdf) (accessed 23.03.2019)
7. M. Edwin, S. Abdulsalam, I. M. Muhammad, *International Journal of Recent Trends in Engineering and Research*, **3**, 5 (2017)

8. R. Parthiban, N. Nagarajan, V. Mahendra Kumaran, D. Senthil Kumar, Journal of Petroleum and Gas Exploration Research, **3**, 3 (2013)
9. C. Patrascioiu, M. Jamali, International Journal of Chemical and Molecular Engineering, **12**, 7 (2018)
10. G. A. Rădulescu, *Proprietățile țițeiurilor românești* (Editura Tehnica, Bucuresti, 1982)
11. C. Patrascioiu, C. Pascu, Revista de Chimie, **60**, 7 (2009)
12. C. Patrascioiu, G. Stamatescu, Revista de Chimie, **66**, 11 (2015)