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Application of the Least Squares Method in the Adjustment of Chlorodifluoromethane (HCFC-142b) Regression Models

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Abstract**—**There are many situations in which human activities have significant effects on the environment. Damage to the ozone layer is one of them. The objective of this work is to use the Least Squares Method, considering the linear, exponential, logarithmic, power and polynomial models of the second degree, to analyze through the coefficient of determination (R^2), which model best fits the behavior of the chlorodifluoromethane (HCFC-142b) in parts per trillion between 1992 and 2018, as well as estimates of future concentrations between 5 and 10 periods, i.e. the concentration of this pollutant in the years 2023 and 2028 in each of the adjustments. A total of 809 observations of the concentration of HCFC-142b in one of the monitoring stations of gases precursors of the deterioration of the ozone layer during the period of time studied were selected and, using these data, the statistical software Excel was used for make the scatter plots of each of the adjustment models. With the development of the present study, it was observed that the logarithmic fit was the model that best fit the data set, since besides having a significant R^2 its adjusted curve was compatible with the natural trend curve of the phenomenon.

Keywords**—**Chlorodifluoromethane (HCFC-142b), ozone (O_3), least squares method, regression models.

I. Introduction

THE ozone layer, located between 15 and 35 km altitude (depending on latitude), is the only natural protection that we have on earth against ultraviolet rays. It is responsible for filtering 95% of UVB rays, which are totally harmful to living things. Ozone (O_3) is a gas (boiling point of -111 ° C) present in small concentrations throughout the atmosphere. Its constitution, about 400 million years ago, allows the development of life in the terrestrial environment, since ozone, a rarefied gas whose molecules are composed of three oxygen atoms, protects the earth from the ultraviolet radiation emitted by the sun [1]. The total amount of atmospheric ozone at any location is expressed in terms of Dobson units (UD), equivalent to the thickness of 0.01 mm of pure ozone, with the density that it would have if it were subjected to sea level pressure (1, 0 atm) and at 0 °C temperature [2]. However, due to the uncontrolled increase in the emission of polluting gases in the atmosphere, originated essentially from the process of world industrialization, the National Aeronautics and Space Administration of the United States (NASA) started the first related alerts to the loss of thickness of the ozone layer between the years of 1979 and 1876 [3]. In addition to this, the studies also indicate the existence of a hole of about 7 million square kilometers over Antarctica. In 1992, NASA identifies a second hole, this time on the North Pole, reaching the regions near the Arctic Circle. In September 1995, the World Meteorological Organization (WMO) reports that the hole on the Antarctic continent already reaches about 10 million km², an area equivalent to the European territory [4].

The ozone layer plays an important role in the biology and climatology of the earth's environment. Radiations below the wavelength of 3000 Å are biologically harmful and ozone helps to filter-out these radiations. The stratospheric ozone layer protects life on earth by absorbing the damaging, high-energy UV-C radiation. Depletion of stratospheric ozone increases the concentration of terrestrial ozone, which is considered harmful for health [5].

Among the main causes of deterioration of the ozone layer, is the chlorine present in the chlorodifluoromethane, which are compounds containing carbon, hydrogen, chlorine and fluorine. Industry and the scientific community see certain chemical substances within this class of compounds as acceptable temporary alternatives to chlorofluorocarbons. CFCs are also found to have health effects which include short-term (acute) and long-term (chronic) effects. Exposure to pressurized CFCs can cause frostbites to the skin and to the upper airway if inhaled. At high temperature, they can degrade to more acutely toxic gases such as chlorine and phosgene. At high concentrations, inhalation of CFCs affects the central nervous system (CNS) with symptoms of alcohol-like intoxication, reduced coordination, light headedness, headaches and convulsions. Disturbances in heart rhythm can occur at very high concentrations and had even caused some deaths from intentional sniffing [6].

The reduction of the ozone layer allows a greater incidence of the ultraviolet rays in the Earth, intensifying the greenhouse effect. This type of radiation is also harmful to any life form on the planet. More than two-thirds of plant species, for example, are damaged with their incidence. In humans, it compromises the immune system's resistance and causes primarily skin cancer and eye diseases, such as cataracts [7]. The United Nations Environment Program (UNEP) calculates that every 1% of destruction in the ozone layer is originated in the world 50 thousand new cases of skin cancer and 100 thousand cataracts [8]. In this regard, studies are needed to

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control emissions of HCFCs into the atmosphere, in particular chlorodifluoromethane (HCFC-142b), which are the most aggressive in terms of the potential for deterioration of the ozone layer.

The objective of this work is to use the Least Squares Method, to analyze through the coefficient of determination (R^2), which model best matches the behavior of the HCFC-142b data set in parts per trillion between 1992 to 2018. In addition, it is intended to make estimates of future concentrations between 5 and 10 periods in each of the adjustment models.

II. The Method of Least Squares

A. Important Aspects

Any set of points in a multidimensional space exhibiting a regular trend can be represented by a mathematical function. Often this function is chosen through an adjustment process known as Least Squares Method or Ordinary Least Squares, which is a mathematical optimization technique that seeks to find the best fit for a set of data trying to minimize the sum of the squares of the differences between the estimated value and the observed data, such differences are called residuals [9]. It is, therefore, an estimator that minimizes the sum of the squares of the regression residuals, in order to maximize the adjustment degree of the model to the observed data.

For the simplest case of a set of points in a two-dimensional space, each point will be represented by x and y coordinates. The mathematical function to be constructed can represent the trend of y as a function of x, $y = f(x)$, or the inverse, with x being represented as a function of y, $x = f(y)$. In other words, one can have y as a dependent variable of x or x as a variable of y [10]. However, one of the fundamental requirements for its application is that the unpredictable factor (error) is distributed randomly and this distribution of data is normal and independent [11].

III. Material and Methods

In order to obtain a considerable margin of confidence in the fit of the regression models of the concentration of chlorodifluoromethane (HCFC-142b) in the period of time studied, a historical survey was made of the largest set of data possible in the *Earth System Research Laboratory* (ESRL), which is the Research Laboratory of the Terrestrial System, coordinated by the United States of America (USA). In this bias, 809 (eight hundred and nine) observations of the concentration of HCFC-142b were selected in one of the monitoring stations of gases precursors of the deterioration of the ozone layer between the years of 1992 to 2018.

With these data, the Excel statistical software was used and applied the Least Squares Method in the following models of adjustments: linear, exponential, logarithmic, power and polynomial of the second degree. Also, the tables of each of the adjustments were made to determine the angular and linear coefficients of the curves fitted to the data set, as well as the coefficient of determination (R^2) to analyze which model best fits the present phenomenon. Finally, the possible concentrations of HCFC-142b between 5 (five) and 10 (ten) periods, i.e. the concentration of this pollutant in the years 2023 and 2028, were verified through the equations of each of the approaches.

IV. Results and Discussion

A. Adjustment Models

Based on the observed data set of chlorodifluoromethane during the time period studied, the graphs of each of the regression adjustment models were made in the Excel statistical software. The following figures denote the behavior of the phenomenon and the adjustment curves for the dataset observed.

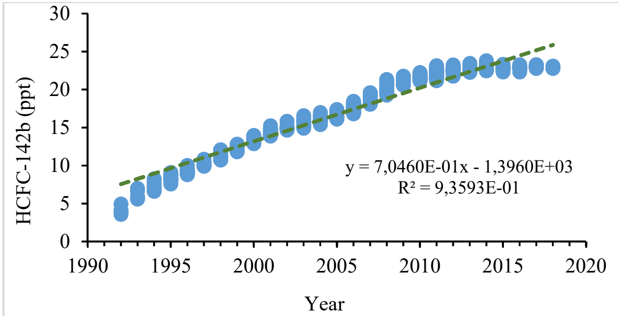

Fig. 1 Linear adjustment

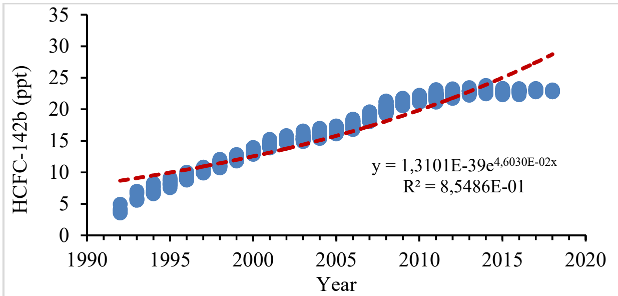

Fig. 2 Exponential adjustment

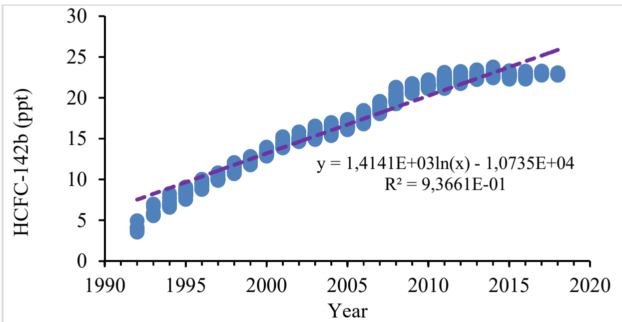

Fig. 3 Logarithmic adjustment

B. Interpretation of the Coefficient of Determination (R^2) of the Adjustment Models

The coefficient of determination or simply R^2, varies between 0 and 1, indicating, in percentage, how much the model can explain the observed values. The coefficient of determination is calculated by (1).

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$$R^2 = \frac{SST}{SSTO} = 1 - \frac{SSE}{SSTO} \quad (1)$$

at where *SSR* is the regression sum of squares, *SSE* is the error sum of squares and *SSTO* is the total sum of squares. Thus, the larger the R^2, the more explanatory the model is, that is, the better it fits the dataset. In this way, we can establish a relation between R^2 and the adjusted curve. Table I shows this relationship.

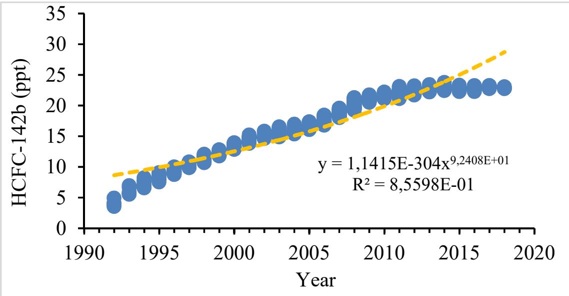

Fig. 4 Power adjustment

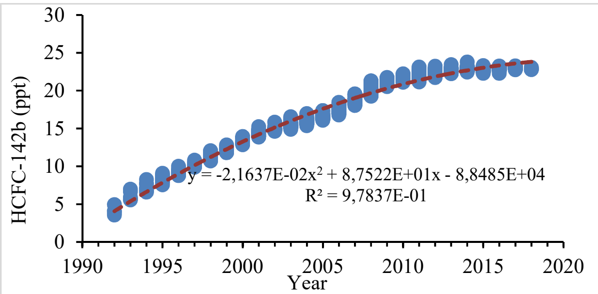

Fig. 5 Second degree polynomial fit

TABLE I
RELATIONSHIP BETWEEN THE R^2 AND THE ADJUSTMENT MODELS

Adjustment Models	Coefficient of determination (R^2)
Linear	0.93592525
Exponential	0.85486262
Logarithmic	0.93661126
Power	0.85598096
Second degree polynomial fit	0.97836982

In the linear adjustment model, R^2 was significant, denoting a reasonable fit to the data set. However, this model is not ideal to represent the observed data, since the adjusted straight line has a behavior different from the natural tendency of the phenomenon, that is, the line tends to grow faster than the concentration level of HCFC-142b in periods futures. On the other hand, in the model of exponential adjustment, R2 was not satisfactory, denoting insufficiency of the model in relation to the fit of the data. On the other hand, in the logarithmic adjustment model the R^2 was considerable and timely, representing a good quality of the model in the adjustment to the data set. In addition, the behavior of the adjusted curve is similar to the curvature of the natural tendency of the phenomenon, thus raising a greater reliability in the future estimates of the concentration of this compound in future periods. Nevertheless, in relation to the model of adjustment by the power function, the R^2 was not significant, indicating a poor quality of the model in the adjustment of the data. In addition, the behavior of the adjusted curve is inversely related to the natural tendency profile of the phenomenon, favoring the occurrence of uncertain extrapolations of the HCFC-142b concentration in future periods. Finally, in the model of adjustment by a polynomial function of the second degree, the R^2 was the most advantageous in terms of quality of adjustment in relation to the other models. However, when it is intended to make future estimates, this model is not preferable, since the adjusted curve is a parabola and at a certain point it will decrease to zero or even negative numbers, which is not compatible with the behavior of the phenomenon in question. Thus, this model is not ideal for representing the behavior of the data, since the concentration of chlorodifluoromethane (HCFC-142b) does not tend to decrease with the passage of time.

C. Future Estimates

TABLE II
LINEAR FIT ESTIMATES

Future Estimates (Year)	Concentration of chlorodifluoromethane (ppt)
2023	29.40348660
2028	32.92647353

TABLE III
ESTIMATES OF EXPONENTIAL ADJUSTMENT

Future Estimates (Year)	Concentration of chlorodifluoromethane (ppt)
2023	36,15309417
2028	45,50908828

TABLE IV
ESTIMATES OF LOGARITHMIC FIT

Future Estimates (Year)	Concentration of chlorodifluoromethane (ppt)
2023	29.36587771
2028	32.85665920
2033	37.72932169
2050	48.11454485

TABLE V
POWER ADJUSTMENT ESTIMATES

Future Estimates (Year)	Concentration of chlorodifluoromethane (ppt)
2023	36.07174129
2028	45.31422026

TABLE VI
ESTIMATES OF THE POLYNOMIAL ADJUSTMENT OF THE SECOND DEGREE

Future Estimates (Year)	Concentration of chlorodifluoromethane (ppt)
2023	24.25754309
2028	23.61886553
2033	21.89835677
2050	7.956529720

In order to know the possible concentrations of chlorodifluoromethane in the years 2023 and 2028, estimates were made in each of the regression adjustment models to

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analyze which model best represents these extrapolations. The following tables denote the concentration content of this organic compound in the estimated periods. In this sense, by analyzing the future predictions of the adjustment models, a continuous increase of HCFC-142b in the terrestrial atmosphere is inferred, causing, in this way, a greater degradation of the hole in the ozone layer. Faced with this frustrating situation, the adoption of public policies by international agencies, such as the World Commission on Environment and Development, is essential to preserve the environment in harmony with the sustainable development of nations. Allied to this, the United Nations - UN, should propose international agreements and socio-environmental campaigns to promote the development of technologies that allow the use of renewable energy sources, as well as to increase industrial production in non-industrialized countries based on technologies ecologically adapted. Once this is done, the world can integrate the environmental issue into economic development, arising not only a new term, but a new way of progressing.

V. CONCLUSION

Based on the analysis of the coefficient of determination (R^2) of each of the adjustment models studied, as well as in the future estimates calculated through their equations, it is concluded that the model that best fit the dataset was the logarithmic, since in addition to having presented a significant R^2 its adjusted curve is compatible with the natural trend curve of the phenomenon, thus guaranteeing a greater reliability in the extrapolations.

The purpose of the present work was the successful application of the Minimum Square Method (MMQ) in adjusting regression models for chlorodifluoromethane (HCFC-142b) from 1992 to 2018.

It is the intention of the researchers of this paper, in future works, to make a study of the adjustment of regression models with a larger dataset, including all the stations of the Earth System Research Laboratory (ESRL), which is the Research Laboratory of the Terrestrial System. In addition, it is intended to consider in future researches the model of hyperbolic adjustment to analyze its behavior in relation to the present phenomenon.

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