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Dynamic Systems Model for Evaluating Atmospheric Greenhouse Gas Emissions in Accordance with USEPA CFR PART 98 Subpart W

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Abstract: The oil industry has a relevant role in the generation of Greenhouse Gases (GHG) in its various segments, among them the Exploration and Production of Oil and Natural Gas (E&P). There are several methodologies for GHG inventories, each with different degrees of uncertainty, which makes the quantification of emissions complex, given the large number of variables to be analyzed. According to the Compendium of Greenhouse Gas Emissions Methodologies for the Oil and Gas Industry of the American Petroleum Institute (API), all GHG emissions should be calculated as a product of an "activity factor" by an appropriate "emission factor". That is, the amount of fuel used, considering how it is used. The product between the activity data and the emission factors provides an estimate of the GHG emissions associated with the company's activities. Based on this premise, this paper presents a model developed in System Dynamics (SD) for the preparation of inventories of CO_2 and CH_4 emissions, the main GHG emitted by the oil industry. The model was developed to meet the requirements of "Subpart W" of the United States Environmental and Protection Agency (USEPA) CFR Part 98, which states that oil and gas E&P facilities that emit at least 25 x 10^3 t CO_2e/year, must report their estimates of total annual GHG emissions, annual individualized emissions of each GHG, and annual individualized emissions of each GHG broken down by source type expressed in metric tons of CO_2e. The proposed model goes beyond the USEPA requirements in that it also allows estimation of emissions of CO_2, of CH_4 and their equivalence in CO_2e from specific sources and groups of sources, generating an estimate of the emissions profile over the entire lifetime of the inventoried facility.

Keywords: Systems Dynamics, Greenhouse Gases, Global Warming, Oil and Natural Gas

1. Introduction

The heating of the Earth's atmosphere is a natural phenomenon and necessary for the maintenance of life on the planet, being caused mainly by the balance between the electromagnetic radiation received by the Earth from the Sun, and the infrared radiation emitted by the Earth back into space. The radiation emitted by the Earth in the form of infrared radiation oscillates around 395 to 400 $W.m^{-2}$, of which about 237 to 270 $W.m^{-2}$ manage to escape through the higher layers of the atmosphere and return to outer space [1]. The balance of this energy balance is retained in the atmosphere, forming the phenomenon that has come to be called the "greenhouse effect", due to the action of various natural and anthropogenic climate forcings, such as insolation, stratospheric aerosols of volcanic origin tropospheric aerosols, water vapor, ozone, halogenated Greenhouse Gases (GHG) [2], land use and land cover change [3], aircraft contrails [4, 5], and of course, among all these, the most relevant are the Greenhouse Gases (GHG).

The GHG include a set of more than 200 compounds of natural and anthropic origin [6], of which the most relevant are carbon dioxide (CO_2), methane (CH_4) and nitrous oxide (N_2O). Such relevance becomes evident if we take into consideration that these three gases alone are responsible for almost 90% of all radiative forcing, the measure of the influence that a factor exerts on the balance of energy input and output in the Earth-atmosphere system, responsible for global warming [7].

In the year 2007, the IPCC released its Fourth Assessment Report on Climate Change (AR4), whose results pointed to various estimates and likely ranges of warming for seven CO_2e stabilization levels: 350 ppm, 1.0°C (0.6°C to 1.4°C); 450 ppm, 2.1°C (1.4°C to 3.1°C); 550 ppm, 2.9°C (1.9°C to 4.4°C); 650 ppm, 3.6°C (2.4°C to 5.5°C); 750 ppm, 4.3°C (2.8°C to 6.4°C); 1,000 ppm, 5.5°C (3.7°C to 8.3°C) and 1,200 ppm, 6.3°C (4.2°C to 9.4°C) [8]. In 2014, the IPCC published the document "Climate Change 2014: Synthesis Report. Contribution of Working Groups I, II and III to the Fifth Assessment Report of the Intergovernmental Panel on Climate Change", where it states that the evidence of human influence on the climate system has grown since its Fourth Assessment Report (AR4). It also states that it is extremely likely that more than half of the observed increase in global average surface temperature from 1951 to 2010 was caused by anthropogenic increases in GHG concentrations and other anthropogenic forcings combined [9].

Eight years have passed since then, in 2022 the IPCC published the document "Climate Change 2022: Impacts, Adaptation and Vulnerability. Contribution of Working Group II to the Sixth Assessment Report of the Intergovernmental Panel on Climate Change", in which it states that since its 2014 report the human influence on global climate change has become unequivocal not only in academia through the increase in scientific publications on the subject, but also in the simple perception of the occurrence of the phenomenon by the lay public. According to the report, current and expected future changes in the climate system indicate the prospect of losses of terrestrial, freshwater, ocean, and coastal ecosystems, including coral reefs in tropical zones. Changes in food security of human populations are also predicted due to degradation of land and water availability, contributing to increased migration and displacement. Consequently, increases in poverty, social inequalities, mortality and morbidity, and mental health problems are also predicted [10].

The growth of atmospheric CO_2 concentrations has been accelerating at sharp and progressive rates, starting from approximately 278 ppm in 1750 [2], reaching 414.71 ± 0.1 ppm by 2021 [11]. In its most recent report, the World Meteorological Organization (WMO) states that concentrations of the 3 major GHGs have reached new highs in 2021, with CO_2 concentrations reaching 415.7 ± 0.2 ppm, CH_4 concentrations reaching 1,908 ± 2 ppb, and N_2O concentrations reaching 334.5 ± 0.1 ppb [12]. These values constitute increases respectively of 149%, 262% and 124% from pre-industrial levels, i.e. before 1750. Since then, in the mid-1800s, with the advent of the Industrial Revolution and the consequent increase in fossil fuel burning, land use change, and agriculture, concentrations of CO_2, CH_4, and N_2O have increased significantly. Such increases in the concentrations of these gases have been altering the Earth's radiative balance, intensifying the natural greenhouse effect, which for millions of years has been the essential support for life on the planet. In 2018, among all industrial sectors, the Energy Sector contributed with about 76.2% of global GHG emissions, which totaled 48.9 x 10^9 t CO_2e. Of this amount, about 1,907 × 10^9 t CO_2e corresponded to emissions from oil and gas extraction, refining and processing activities, including emissions from Exploration and Production (E&P) activities [13].

In 2021, GHG emissions related to the Energy Sector will total 36.6 x 10^9 t CO_2e, which corresponds to the largest historical annual increase, reflecting the strong economic recovery in the post COVID-19 period and the mismatch of the Nationally Determined Contributions (NDCs) and the non-compliance with the national emission reduction targets established by the Paris Agreement [14]. In the period between the years 1965 and 2018, the 20 largest GHG emitting companies, the so-called "Carbon Majors" totaled an emissions volume of 493,471 × 10^9 t of CO_2 and of CH_4 [15]. Over a broader time horizon, in the period 1854-2015 this group of companies was responsible for the emission of 923 × 10^{12} t (Gt) of CO_2e, which represents more than half (52%) of global industrial GHG emissions since the beginning of the industrial revolution [16]. These numbers demonstrate the relevance of the Energy Sector in global GHG emissions and the importance of creating and implementing strategies that allow the reduction of its emissions.

This scenario demonstrates the importance of developing initiatives and tools that allow companies to develop strategies to mitigate their GHG emissions. It is well known that the sector with the highest contribution to GHG emissions is the Energy Sector, which includes the activities of Exploration and Production (E&P) of Petroleum and Natural Gas [17]. Although there is no global consolidated data regarding the specific emissions of E&P activities, the relevance of assessing these emissions is evident when we look at the 2021 report of the Greenhouse Gas Reporting Program (GHGRP) [18]. Among other requirements, the GHGRP requires reporting of emissions and relevant information from major GHG emission sources, which serve for tracking and comparisons between emission sources, as well as identifying opportunities to reduce emissions, minimize energy waste, and climate policy development. The GHGRP is subdivided into 47 subparts, each covering different industrial sectors, which are required to report their GHG emissions if they exceed 25,000 metric tons of CO_2e.

In its subpart W, the GHGRP focuses on emissions from Oil and Natural Gas systems for Onshore Production, Offshore Production, Gathering and Boosting, Natural Gas Processing, Natural Gas Transmission Compression, Natural Gas Transmission Pipeline, Underground Natural Gas Storage, Liquefied Natural Gas (LNG) Import/Export, LNG Storage, Natural Gas Distribution, and Other Oil and Gas Combustion. In the year 2021, the GHGRP report showed emissions from 2379 facilities among the above 10 categories, which reported total emissions of 312.2 x 10^6 t CO_2e. These emissions were formed from the emissions of 241 x 10^6 t CO_2 and in CO_2, 71 x 10^6 t CO_2 and in CH_4 and 0.2 x 10^6 t CO_2e in N_2O, respectively 77.19%, 22.74% and 0.07% of the total emissions [18]. The model presented in this work had its conceptual planning based on the requirements of "Subpart W" of the USEPA CFR Part 98 Regulation, being adaptable to any of the systems listed in subpart "W", needing the definition of specific emission sources and their respective emission and activity factors to facilitate the realization of inventories of GHG emissions from E&P activities, and determine the relevance of each variable or set of variables (Activity and Emission Factors, isolated emission sources or groups of sources, origin of emissions, types of gases), as well as the effect that changes in each one of them will have on the system as a whole, so that the information obtained about changes in the project will allow better quality decisions to be made.

The main objective of this work is to present the development of a mathematical model based on the System Dynamics (SD) language, through which it is possible not only the quantification of emissions, but also to determine how they occur in each of the emission sources in Oil and Gas Exploration and Production facilities. This type of modeling allows the determination of the exact role of each variable in the change in the system's behavior at each change made in its variables. This characteristic allows the adoption of appropriate policies to achieve the goals pre-defined by the modeler, even if these goals should only be achieved over longer time horizons.

2. Methodology

2.1. System Dynamics

System Dynamics was developed in the 1950s at the Massachusetts Institute of Technology (MIT), by Jay Wright Forrester, and was consolidated in his work "Industrial Dynamics", published in 1961 [22], to study the relationships and influences existing between the elements of a system, whether it is a corporation, a natural ecosystem, an industrial plant, an oil platform or a living organism, for example. It uses modeling as a tool, through which it seeks to reproduce the structure of the cause-and-effect relationships between the elements of a system, and simulation, which analyzes how these structures behave over time [22]. Its greatest benefit is that it allows one to evaluate the best options for achieving desired results and avoiding undesired ones by manipulating each part, evaluating its influence on the structure. As an effect, it is possible to test decisions, evaluate their results, and correct in advance the necessary directions to achieve the expected results.

In the origin of the development of System Dynamics, the elaboration of models was based on the simple concepts of Stocks, Flows, Converters and Connectors [23]. The difficulty then prevailing of writing computer programs where a large number of equations were present generated the need for a simplification of the equations used in modeling, in order to simplify the visualization of what was being modeled. This concept gave rise to what is known to this day as "The Language of Flows and Inventories". Understanding the concepts of stocks and flows is essential to the construction of flow diagrams [24].

Stocks represent variables that can be several physical units, such as position, velocity, force, mass, work, energy, among others [25]. They are state variables that demonstrate the situation of the System over time [26]. The stocks represent the accumulation of the results of the system's actions, that is, they are the current values of the variables, resulting from the accumulated difference between the input and output flows [27]. Flows are control variables that represent the rates of change in the state of a stock-type variable over time. For this reason, flows are always linked to stocks that represent that variable. Flows can relate to stocks as inflows or outflows, causing stock values to increase or decrease [26]. Their direction of action can occur either unidirectionally or bidirectionally, representing then in relation to the stocks connected to them respectively inflows or outflows and inflows and outflows. Flows can represent physical units such as velocity, acceleration, force, power, among others [25]. The clouds represented at the beginning and end of each flow represent source and final destination elements outside the boundaries of the system under analysis, which are not being considered.

In addition to Flows and Stocks, the fundamental blocks of the Systems, auxiliary elements are used to formulate the data in order to define the equations of the flows. They serve to combine through algebraic operations the flows, stocks, and other auxiliary elements. They are used to model the information, not the physical flow, and can be changed instantaneously, without delay [28]. The auxiliary elements besides being responsible for performing algebraic operations also represent sources of information external to the system:

1. Converters: Converters can be used either as constant values or as functions. As functions, they convert the values of a variable according to a user-defined equation. They display the rates that modify and lend values to streams and are represented by means of circles [29, 30]. Converters can perform different tasks, such as setting values for constants, defining external inputs to the model, calculating algebraic relationships between values, serving as a repository for graph functions [26].
2. Connectors: Connectors serve to establish a relationship between two components in the construction of the diagram, representing the passage of information between the variables that will form the mathematical expressions used in the model [26, 29, 30];
3. "Delays": "Delays" are next to the concept of "feedback" the ones responsible for much of complex systems. "Delays are the result of an action that produced different effects in time and space. In feedback, the feedback can occur with a delay in relation to the variables involved, generating

unexpected behavior. This delay occurs when the effects of a variation in one of the elements of the system do not occur immediately, causing undesired effects, such as oscillations or amplifications [33].

Figure 1 shows the building blocks and auxiliary elements used in the modeling.

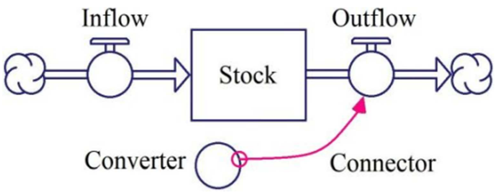

Figure 1. *Building blocks and auxiliary elements used in System Dynamics.*

Dynamic systems modeling is a high-value mathematical tool that has been used in diverse areas of knowledge in areas as diverse as energy planning [32], transition to low carbon intensity [33], biogas production [34] transportation systems [35], telecommunications [36], marketing policies and strategies [37], retirement systems [38], hydrological processes [39], public health [40], urban mobility [41], neurology [42], tourism [43], construction waste [44], carbon footprint [45].

2.2. API Compendium and USEPA CFR Part 98 Subpart W

There are several methodologies used for estimating atmospheric GHG emissions. The present work was based on the last two versions of the "API Compendium of Greenhouse Gas Emissions Estimation Methodologies for the Oil and Gas Industry" [20, 21], which is the final result of a long discussion process conducted by a Working Group formed by the American Petroleum Institute (API), its various associated companies, governments and non-governmental organizations. This Working Group evaluated and documented a series of calculation techniques, several existing protocols, and useful emission factors for the development of GHG emission inventories in order to elaborate common methodologies and ensure a broad review of their efforts. For the preparation of the "Compendium", the following documents were analyzed:

1. Australian Greenhouse Office (AGO), Workbook for Fuel Combustion Activities;
2. Australian Petroleum Production and Exploration Association (APPEA), Greenhouse Challenge Report;
3. Canadian Association of Petroleum Producers (CAPP), Global Climate Change Voluntary Challenge Guide;
4. Canadian Industrial Energy End-Use Data and Analysis Center (CIEEDAC) memorandum on "Guide for the Consumption of Energy Survey";
5. Environmental Protection Agency (EPA) Emission Inventory Improvement Program;
6. Exploration and Production Forum (E&P Forum) Methods for Estimating Atmospheric Emissions from E&P Operations;
7. Gas Technology Institute (GTI), GRI-GJGCalc'Version 1.0;
8. Intergovernmental Panel on Climate Change (IPCC), Guidelines for National Greenhouse Gas Inventories;
9. Regional Association of Oil and Natural Gas Companies in Latin America and the Caribbean (ARPEL), Atmospheric Emissions Inventories Methodologies in the Petroleum Industry;
10. UK Emissions Trading Scheme;
11. World Resources Institute and World Business Council for Sustainable Development, The Greenhouse Gas Protocol.

The methodologies presented in the Compendium can be used to guide the estimation of GHG emissions for individual projects, entire facilities (such as oil platforms), or corporate inventories. The methodologies are more focused on carbon dioxide (CO_2) and methane (CH_4) emissions since such compounds are the relevant GHGs for the oil and gas industry [46].

2.3. Calculation of GHG Emissions from Emission and Activity Factors

The present work used for calculation methodology the emission factors available in literature according to API [20, 21], Based on:

1. Easy data acquisition;
2. Simplicity in its application;
3. Quick model update in case of factor updates;
4. Full adaptation to the objectives of the model.

The calculation of emissions based on emission factors is done based on the products between the various emission factors (EF) corresponding to each of the specific sources inventoried and their corresponding activity factors (AF), as described in Equation 1. An inventory is the sum of emissions from all emission sources of a facility or corporation, as described in Equation 2 [20, 21].

$$Emissions\ Source_i = EF_i\ x\ AF_i \qquad (1)$$

$$Emissions\ Inventory = \sum_{i=1}^{\#\ of\ sources} EF_i\ x\ AF_i \qquad (2)$$

Emission Factors represent a "typical" or "average" emission rate of the mass of GHG emissions per unit of activity, whereas Activity Factors are generally measured values that represent any action or operation that influences GHG release such as counting the number of equipment that are emission sources or the amount of fuel consumed [19, 20, 47].

After quantifying the GHG emission volumes from each specific source by applying Equation 1, it is necessary to equalize them to the radiative forcing of CO_2. For this, the Global Warming Potential (GWP) of CO_2 and CH_4 is used as the basis of the common metric, as shown in Table 1 [10].

Table 1. *Global Warming Potential of CO_2 e do CH_4.*

GHG	GWP
CO_2	1
CH_4	28

The emission of CO_2e is obtained by multiplying the GHG emission by its corresponding GWP. Since the inventory is the summation of a mixture of several GHGs, the total CO emission2 e is the sum of the emissions converted to CO_2e of each GHG, according to Equations 3 and 4.

$$GHG_i\ emissions\ (CO_2e) = GHG_i\ emission\ x\ GWP_i \quad (3)$$

$$Total\ emissions\ GHG\ (CO_2e) = \sum_{i=1}^{\#\ of\ GHG} GHG_i\ emissions\ (CO_2e) \quad (4)$$

3. Results and Analysis

3.1. Regulation 40 CFR Part 98 "Mandatory Reporting of Greenhouse Gases: Petroleum and Natural Gas Systems; Final Rule

In the year 2010 the US environmental agency (USEPA) promulgated its regulation 40 CFR Part 98 "Mandatory Reporting of Greenhouse Gases: Petroleum And Natural Gas Systems; Final Rule". Such regulation states that operators and owners of facilities that emit at least 25 x 10^3 t CO_2 and per year must report emissions from all sources located at the facilities according to the methods defined in the regulation [19]. In its item "II. Reporting Requirements for Petroleum and Natural Gas Systems - D. Summary of the Requirements for Petroleum and Natural Gas Systems (Subpart W)", defines that the term "Offshore petroleum and natural gas production" used in the regulation is applicable to any temporary or permanent platforms used for extraction of hydrocarbons and their processes and treatments for transferring the hydrocarbons to transport vessels or to land. In addition, offshore production includes secondary platforms connected to the main platform by means of gangways, as well as storage tanks associated with the platform structure, and FPSO's. This category does not include reporting of emissions from drilling and exploration that is not performed on offshore production platforms.

On April 12, 2010, the USEPA proposed "Subpart W," an amendment to 40 CFR Part 98, changing the requirements for the Greenhouse Gas Reporting Program (GHGRP). Under this amendment, offshore platforms must report the following emissions [48]:

1. CH_4 from the identified equipment (Amine Units, Boilers/Heaters/Burners, Diesel and Gasoline Engines, Drilling Rigs, Combustion Flares, Fugitives, Glycol Dehydrators, Losses from Flashing, Mud Degassing, Natural Gas Engines, Natural Gas Turbines, Pneumatic Pumps, Pressure/Level Controllers, Storage Tanks and Cold Vents) in the 2008 edition of the "Gulfwide Offshore Actvities Data System" (GOADS), with the exception of their emissions from combustion equipment [49];
2. CO_2, CH_4 and N_2O from the flares;
3. CO_2, CH_4 and N_2O from stationary combustion sources such as boilers, heaters, burners, gasoline, diesel or natural gas engines, natural gas, diesel or "dual fuel" turbines.

Facilities regulated by "Subpart W" must report the following information:

1. Total annual GHG emissions, expressed in metric tons of CO_2e;
2. Individualized annual emissions of each GHG, expressed in metric tons of CO_2e;
3. Individualized annual emissions of each GHG, expressed in metric tons of CO_2 and broken down by source type.

In order to meet the requirements of "Subpart W" of the USEPA CFR Part 98 Regulation, the model developed was based on the GHG emission sources presented in Table 2-1 of the API Compendium [20]. The 43 sources listed are distributed among sources that can be specific to exploration or production facilities or can be common to both activities. Such sources are further divided into four major emission source groups:

1. Emissions from combustion;
2. Fugitive emissions;
3. Emissions from the ventilation processes;
4. Emissions from indirect sources.

The volume of GHG emitted by the E&P sector varies based on several different parameters, such as reservoir characteristics, field age, production techniques adopted, regulatory issues, emission control practices, oil API grade, with the largest volumes, around 70 to 75% of emissions, coming from the combustion of fossil sources for self-generation of energy. Also relevant in the upstream are the CO_2 emissions from flaring, and CH_4, from venting sources. Emissions of N_2O are also reported, but in low volumes, and can be discarded [50].

Based on the assumptions presented, the 43 sources listed [20] were reduced to the 13 sources listed in Table 2, the main combustion and ventilation sources were selected, and the fugitive emission sources were discarded.

Table 2. *Fonts selected for the model.*

Sources groups / Sources	Combustion	Ventilation
Stationary Devices / Boilers/steam generators	x	
Stationary Devices / Dehydrator reboilers	x	
Stationary Devices / Heaters/treaters	x	
Stationary Devices / Internal combustion (IC) engine generators	x	
Stationary Devices / Flares	x	
Mobile Sources / Mobile drilling equipment	x	
Process Vents / Dehydration processes		x
Process Vents / Dehydrator Kimray pumps		x
Process Vents / Gas sweetening processes		x
Other Venting / Exploratory drilling		x

Sources groups / Sources	Combustion	Ventilation
Other Venting / Well testing and completion		x
Maintenance/Turnarounds / Well completions		x
Maintenance/Turnarounds / Well unloading and workovers		x

3.2. Definition of the Emission and Activity Factors

In developing a practical application of the model, one must take into account the objectives of the inventory to be developed, so that the choice of a more precise approach than the adoption of Emission Factors collected in literature can be replaced by more accurate approaches. In this regard, an important issue to be taken into consideration is the direct relationship between quality and cost of information, as represented by Figure 2. The adoption of literature-derived emission factors has the advantage of simplicity and low cost but exacts its price by increasing the uncertainty of the accuracy of the data used and consequently the lower quality of the final results. On the other hand, the continuous monitoring of emissions would have a high cost, but accompanied by greater accuracy and precision [20, 21].

The uncertainty arising from the measurement methods used to determine the accuracy of the emission factors is an aspect that can change the degree of accuracy in emissions estimates. The accuracy of the measurement method used depends on the technological resources available, the desired accuracy, and the costs involved.

Once the emission sources were selected and having already defined as calculation methodology the use of emission factors available in literature according to API [20, 21], we started to search in literature the emission and activity factors corresponding to the selected sources. Tables 3 and 4 below summarize the selected Emission Factors (EF) and Activity Factors (AF).

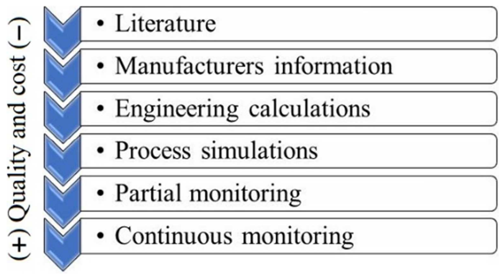

Figure 2. *Types of approach for estimating GHG emissions.*

Table 3 presents the AF and FE selected from the research [20] (Tables 4-12, 5-2, 5-5, 5-23, 8-8, 8-28, 8-30, Exhibit 5.30), [51] (Tables 4-9 and B-2.0), [52] (Tables VI-2, VI-3 and V-17), [53-55] (Table 1.4-2), for the calculation of CO_2 emissions.

Table 4 presents the FA and FE selected from the same sources, for the calculation of CH_4 emissions.

Table 3. *Activity Factors (AF) and Emission Factors (EF) used to calculate emissions from* CO_2.

Source groups / Sources	AF	Value	EF	Value	Combustion	Ventilation
Stationary Devices / Boilers/steam generators	AF1	4,00E+05	EF1	1,92E-03	x	
Stationary Devices / Dehydrator reboilers	GP	Produced gas	EF2	2,80E-02	x	
Stationary Devices / Heaters/treaters	AF2	4,00E+05	EF3	1,92E-03	x	
Stationary Devices / Internal combustion (IC) engine generators	AF3	6,06E+02	EF4	2,64E-06	x	
Stationary Devices / Flares	GQ	Burnt gas	EF5	1,40E+00	x	
Mobile Sources / Mobile drilling equipment	AF4	7,71E+01	EF6	2,64E+00	x	
Process Vents / Dehydration processes	x	X	x	x		x
Process Vents / Dehydrator Kimray pumps	x	X	x	x		x
Process Vents / Gas sweetening processes	GP	Produced gas	EF7	3,90E-03		x
Other Venting / Exploratory drilling	AF5	4,00E+00	EF8	2,80E-08		x
Other Venting / Well testing and completion	AF6	3,00E+00	EF9	3,32E+00		x
Maintenance/Turnarounds / Well completions	FA7	6,00E+01	FE10	7,30E+00		x
Maintenance/Turnarounds / Well unloading and workovers	FA8	5,00E+00	FE11	7,30E+00		x

Table 4. *Activity Factors (AF) and Emission Factors (EF) used to calculate emissions from* CH_4.

Source groups / Sources	AF	Value	EF	Value	Combustion	Ventilation
Stationary Devices / Boilers/steam generators	AF9	4,00E+05	EF1	1,92E-03	x	
Stationary Devices / Dehydrator reboilers	GP	Produced gas	EF2	2,80E-02	x	
Stationary Devices / Heaters/treaters	AF10	4,00E+05	EF3	1,92E-03	x	
Stationary Devices / Internal combustion (IC) engine generators	AF11	6,06E+02	EF4	2,64E-06	x	
Stationary Devices / Flares	GQ	Burnt gas	EF5	1,40E+00	x	
Mobile Sources / Mobile drilling equipment	AF12	7,71E+01	EF6	2,64E+00	x	
Process Vents / Dehydration processes	GP	X	x	x		x
Process Vents / Dehydrator Kimray pumps	GP	X	x	x		x
Process Vents / Gas sweetening processes	GP	Produced gas	EF7	3,90E-03		x
Other Venting / Exploratory drilling	AF13	4,00E+00	EF8	2,80E-08		x
Other Venting / Well testing and completion	AF14	3,00E+00	EF9	3,32E+00		x
Maintenance/Turnarounds / Well completions	AF15	6,00E+01	EF10	7,30E+00		x
Maintenance/Turnarounds / Well unloading and workovers	AF16	5,00E+00	EF11	7,30E+00		x

Among all GHG listed in the Kyoto Protocol, the two GHG that must be included in inventories are CO_2 and CH_4, given their relevance to the overall emissions of the sector of Exploration and Production of Petroleum and Natural Gas [20, 21]. In fact, as an example to corroborate this statement, we can take as an example of emissions profile, the emissions of CO_2, CH_4 and N_2O emitted by PETROBRAS, one of the largest oil companies in the world, in the period between the years 2015 and 2021 [56]. In this period its annual N_2O emissions do not even reach 1% of its total emissions as observed in Figure 3, which characterizes the low relevance of N_2O emissions in the E&P sector. Thus, although [48] suggests the inclusion of N_2O emissions from flares and stationary combustion sources, the present model deals specifically with CO_2 and CH_4 emissions.

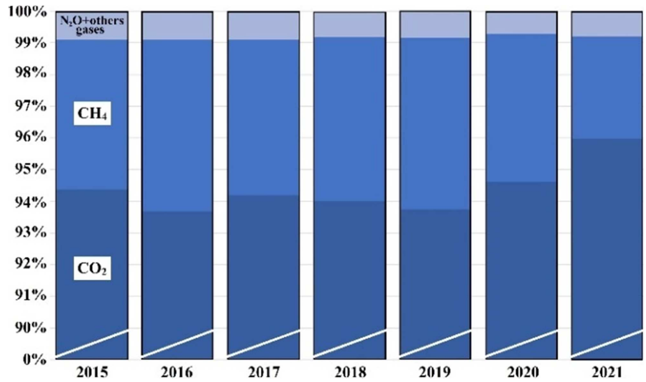

Figure 3. PETROBRAS CO_2, CH_4 and N_2O emissions in the period 2015 to 2021.

As previously mentioned, there are several methodologies available for the preparation of GHG emissions inventories. The choice of the methodology presented by the API Compendium is due to the fact that in practice the Compendium should be understood as much more than a specific methodology. The API Compendium is the result of a work developed by several global institutions such as API and IPIECA (International Petroleum Industry Environmental Conservation Association), specialized in oil and gas. This specificity gives the API Compendium a degree of specialization that distinguishes it from other protocols available today for conducting GHG emissions inventories. The use of the API Compendium allows not only the use of a methodology sufficiently accepted by the market, but also a clear definition of the various sources of emissions existing in the Exploration & Production segment, the object of the model proposed here.

According to API [20, 21] the emissions for a specific source are calculated as the product between the Emission Factor (EF) of the source and an Activity Factor (AF). An inventory corresponds to the sum of all emissions from a facility or company, as per Equation 4.

From the 43 emission sources listed in Table 2-1 of the API Compendium [20], 13 of them were selected, representing the two main groups of emission sources, combustion and ventilation, responsible for about 80% of the total GHG emissions. Their Emission Factors (EF) and Activity Factors (AF) were collected from several bibliographic sources and listed in Tables 3 and 4. The output values for annual emissions presented in the tables mentioned above are presented in t/year, in order to standardize the information that serves as a basis for feeding the model. However, the information available in the literature is presented in various metric standards, sometimes using the International System (SI), sometimes using the English System, which is more widely adopted in the USA. Due to this characteristic, all the FE and AF needed to be standardized to the SI and converted to t/year. For this, the "The International System of Units (SI), 2019 Edition" from the National Institute of Standards and Technology [57] was used as support.

Once the FE and FA were obtained and duly converted to a common base in t/year, for the conversion of CO_2 and CH_4 emissions to CO_2e emissions, the Global Warming Potential (GWP) values of 1 and 28 respectively were used, as presented in Table 1 [10]. Finally, emissions were calculated based on a hypothetical production curve of a Natural Gas Production Field with an estimated lifetime of 30 years as presented in Table 5, and these daily volumes were converted to annual volumes, and only then used in the model.

Table 5. *Volumes of natural gas produced and flared, in 10^6 m^3/day.*

Year	Produced gas	Burnt gas	Year	Produced gas	Burnt gas
2023	0,57	0,24	2038	3,80	0,38
2024	3,32	0,70	2039	3,85	0,33
2025	6,52	0,65	2040	3,95	0,25
2026	6,85	0,69	2041	4,00	0,31
2027	5,80	0,50	2042	4,00	0,33
2028	5,50	0,35	2043	3,80	0,38
2029	3,80	0,29	2044	3,00	0,29
2030	3,00	0,25	2045	2,85	0,28
2031	2,10	0,21	2046	2,80	0,23
2032	1,84	0,18	2047	2,40	0,24
2033	1,65	0,16	2048	2,00	0,20
2034	1,80	0,15	2049	1,40	0,14
2035	2,50	0,13	2050	0,60	0,05
2036	2,95	0,12	2051	0,40	0,05
2037	3,60	0,36	2052	0,20	0,03

3.3. Model Building

3.3.1. The iThink Computational Tool

The construction of a System Dynamics Model has at its disposal a series of computational tools represented by a wide variety of programs for its execution, each with its own characteristics and approaches. According to the website of the System Dynamics Society (http://www.systemdynamics.org/), the three main commercial software programs currently available are as follows:

1. iThink/STELLA (http://www.iseesystems.com/): iThink and STELLA are two names for the same model development platform, differentiated by the modeling objectives. While STELLA is for education and

research, iThink is for policy and business modeling. The model presented in this paper was developed in iThink software;
2. Powersim Studio (http://www.powersim.com/): Powersim Studio is available in different configurations, available under commercial and academic licenses;
3. Vensim (http://vensim.com/): Vensim is available under commercial and free licenses for educational purposes, in which case a version with limited features is available.

Besides these, several other programs are available under commercial licenses, as well as free and even open-source licenses. Among these are the following:

1. AnyLogic, produced by AnyLogic Company (http://www.anylogic.com/);
2. Smia, produced by Dynaplan (https://www.dynaplan.com/?message);
3. GoldSim, produced by The GoldSim Technology Group (http://www.goldsim.com/Home/);
4. Berkeley Madonna, produced by the University of California at Berkeley (http://www.berkeleymadonna.com/);
5. Simile, produced by Simulistics from the University of Edinburgh (http://www.simulistics.com/).

Programming in the iThink software is object-oriented, which are symbolized by icons representing variables with specific functions (stocks, flows, converters, and auxiliary variables), which visually describe the mathematical model defined to represent the real phenomenon under study. In iThink's modeling environment, the modeler does not deal directly with the differential equations intrinsic to the program but establishes the relationships between the variables present in the system under study [58]. Thus, the elaboration of the model began with the definition of the variables involved, in order to correctly fit them into their variable category. Based on this premise, each source of GHG emissions was treated as a flow, the groups of sources were treated as stocks, and the Emission Factors, Activity Factors, and the production and gas flaring curves were considered as auxiliary variables. In the model are represented all GHG emission sources and all Emission and Activity Factors presented in Tables 3 and 4, the Produced Gas and Burnt Gas curves presented in Table 5, and the GWP factors of CO_2 and CH_4 as per Table 1 [10], to totalize the emissions in CO_2e.

3.3.2. Application of Activity and Emission Factors

Each selected source is related to its respective Activity and Emission Factor as presented in Tables 3 and 4, or to its respective volumes of produced or flared gas, as presented in Table 5. The calculation of the CO_2 or CH_4 emission volumes from each source is done through the product between its Emission Factor (EF) and its corresponding Activity Factor (AF), as presented in Equation 1. Once these GHG volumes are totaled according to Equation 2, their corresponding GWP, presented in Table 1, are applied to the totalized volumes of CO_2 or CH_4, determining their equalization to the CO_2 radiative forcing, therefore already presenting their volumes in CO_2e according to Equation 3. Finally, in order to total the GHG emissions of all sources already equalized in CO_2e, the sum of CO_2 and CH_4 emissions already converted to CO_2e is made according to Equation 4.

3.3.3. Structure of the Model

The model presented allows not only the precise determination of the participation of each source in the global calculation of emissions, but also the behavior of their emissions throughout the evaluated period of time. This allows a previous evaluation of the actions that may be necessary for emission mitigation processes, either by company's own policy or due to legal regulations that may impact the company's activities.

Observing Figure 4, we see that the model layout was developed by dividing it into 4 sectors, each of which concentrates the emissions in its 4 outflows, corresponding to:

1. Sector 1: total CH_4 emissions from ventilation, converted to CO_2e;
2. Sector 2: total CH_4 emissions from combustion, converted to CO_2e;
3. Sector 3: total CO_2 emissions from ventilation, converted to CO_2e;
4. Sector 4: total CO_2 emissions from combustion, converted to CO_2e.

"Subpart W", of 40 CFR Part 98 regulations [48] requires platforms that emit at least 25,000 tons of CO_2e per year to report the following emissions:

1. Total annual GHG emissions, expressed in metric tons of CO_2e, represented by the sum of the emissions of the four sectors;
2. Individual annual emissions of each GHG, expressed in metric tons of CO_2e, represented by the sum of the emissions of the 1st and 2nd sectors to represent CH_4 emissions, and by the sum of the emissions of the 3rd and 4th sectors to represent CO_2 emissions;
3. Individual annual emissions of each GHG, expressed in metric tons of CO_2e and broken down by source type, represented by the sum of emissions from the 1st and 3rd sectors to represent emissions from ventilation, and the sum of emissions from the 2nd and 4th sectors to represent emissions from combustion.

In each sector, the initial flows represent the CH_4 or CO_2 emissions from ventilation or combustion, according to their specific sector. In order to calculate the emissions from each source, the Activity Factors (AF) and Emission Factors (EF) are included through converters connected to each of the flows in order to start the inventory according to Equation 1. The converters are switch type controls that allow the inclusion or not of emissions from each specific source in the inventory. Thus, each specific source can have its emissions evaluated, either individually or together with any other, at the modeler's discretion.

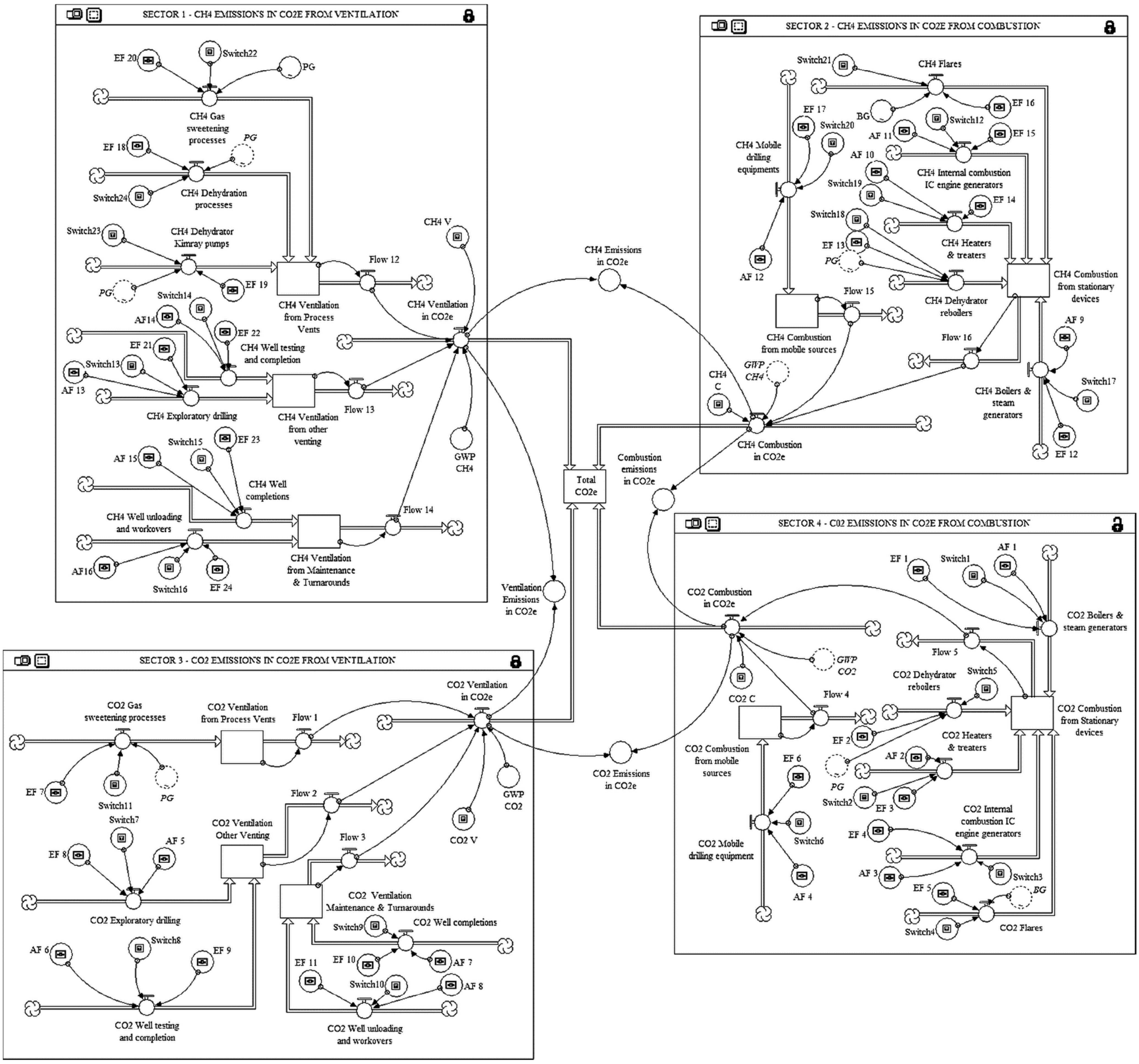

Figure 4. *Model developed to calculate atmospheric GHG emissions.*

The flows are concentrated in partial stocks, which represent the emissions of CH_4 or CO_2 by group of ventilation sources. The flows from each stock are concentrated into a single outflow of the sector, representing the total emissions of CH_4 or CO_2 from ventilation or combustion, according to the sector. The product of such emissions by their corresponding GWP (Global Warming Potential) allows obtaining the emissions duly converted to CO_2e. The GWP relativizes the atmospheric concentrations, residence times and radiative forcing of each GHG with the same parameters of CO_2, making it possible to equalize the calculation of the atmospheric effects of each non-CO_2 GHG.

This index, called carbon dioxide equivalent (CO_2e), represents the mass of CO_2 that would need to be emitted instead of the non-CO_2 emitted GHG, sufficient to cause the same impacts on the climate system. The CO_2 equivalent emission is obtained by multiplying the GHG emission by its corresponding GWP, as shown in Equation 3. If a mixture of several GHG is being evaluated, as occurs in the model presented here, the total CO_2e emission will be the sum of the emissions already converted to CO_2e of each GHG, as shown in Equation 4.

The model was developed in such a way that the requirements listed by "Subpart W" of the USEPA Regulation 40 CFR Part 98 [48] were fully met. Thus, the model allows to present the estimated total annual GHG emissions expressed in metric tons of CO_2e, the individualized annual emissions of each GHG expressed in metric tons of CO_2e, and the individualized annual emissions of each GHG expressed in metric tons of CO_2e and broken down by source type.

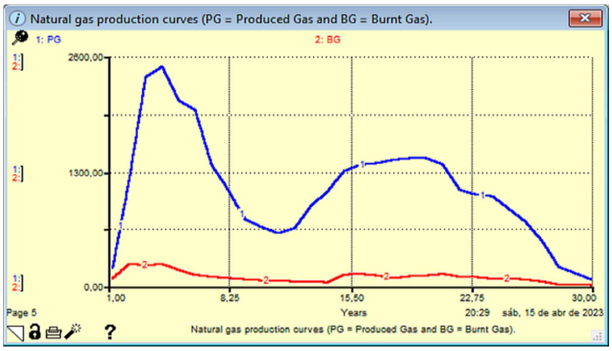

Figure 5. *Produced Gas (PG) and Flared Gas (FG) curves over the 30 years of the simulation.*

Of the 13 sources of GHG emissions included in the model, 5 of them use the natural gas production and flaring curves for calculating their CH_4 emission estimates and 3 of them for CO_2. The production and flaring curves presented in Table 5 were entered into the model as floating variables over the 30-year simulation period (Figure 5).

In models produced in the iThink software, the manipulation of variables, stocks and flows included is performed through a "Control Panel", a graphical interface where input and output information are presented, besides graphs and tables where the simulation results are presented. This graphical interface is totally flexible and can be built by the modeler according to the information that is of his interest to present. Besides this flexibility in its assembly, the "Control Panel" allows the manipulation of each variable or group of variables, changing the values assigned to each of them, and consequently changing the simulation results. Figure 6 shows the "Control Panel" developed for the model.

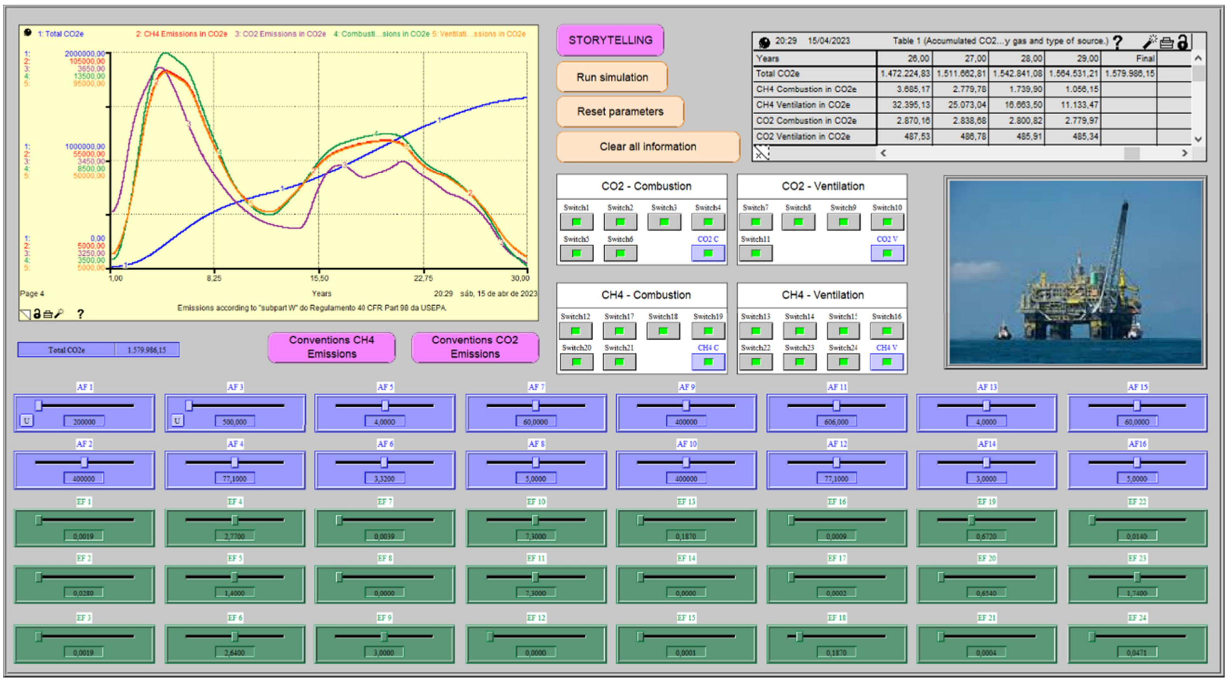

Figure 6. *Control Panel developed for the 30 years simulation.*

In the "Control Panel" of the model, several controls can be observed, each with specific functions:

1. Slider controls (Figure 7): allow to change the values set for each of the variables represented by this type of control. In the model presented, the sliders represent each Activity Factor and each Emission Factor presented in Tables 3 and 4. Their amplitude limits can be set at the modeler's discretion, so that new values for the specific variable can be changed without changing the model. This means that real changes in the Emission Factors or Activity Factors of the inventoried installations can be reproduced in the model at any time.
2. Switches (Figure 8): controls that "turn on" or "turn off" the participation of one or more variables in the calculation of emissions. In the model, each source of emissions presented in Tables 3 and 4 has been connected to a switch, so that each specific source can be included or excluded in the emissions estimate. This allows the emissions from each source to be estimated individually, determining their relevance among the total emissions.

Figure 7. *Sliders.*

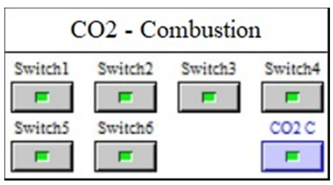

Figure 8. *Switches.*

One of the great differences of the model is its ability to present a thorough level of detail in the emissions profile, given its adjustable ability to profile emissions even from specific sources, as represented by Figure 9, which represents the emissions profile of CO_2, CH_4 and total CO_2e exclusively from Flares over the 30-year simulation. Just as the specific emissions from flares have been calculated and graphically represented, any other source or group of emission sources can also be graphically represented.

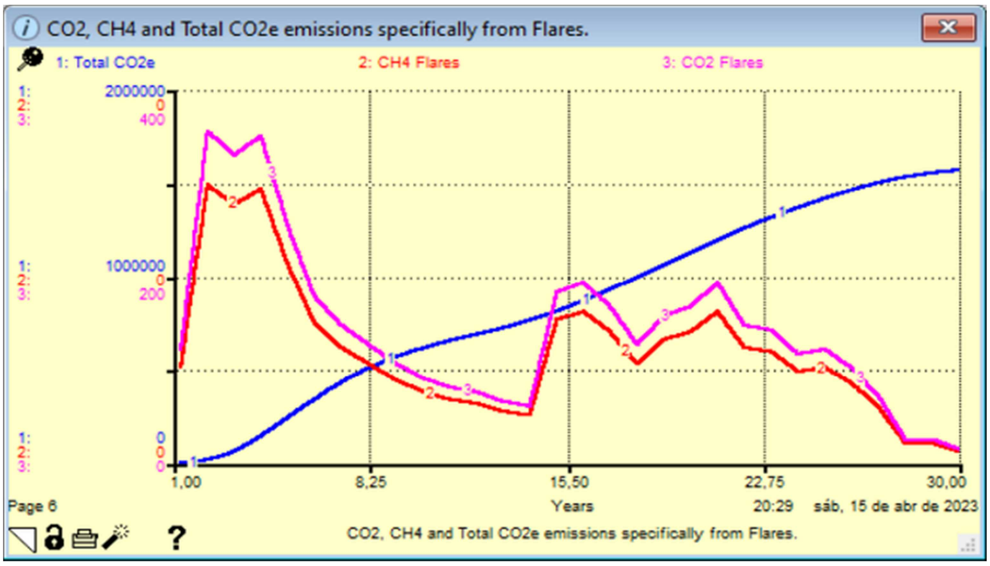

Figure 9. *Profile of CO_2, CH_4 and CO_2e emissions exclusively from Flares over the 30 years of the simulation.*

Each graph, whether it refers to a single source of emissions, a group of sources, or total emissions, can be accompanied by its respective data table, presenting the emission volumes for each stipulated time period, as presented in Figure 10.

16:57 12/04/2023 Table 1 (Accumulated CO2...y gas and type of source.)

Years	26,00	27,00	28,00	29,00	Final
Total CO2e	1.489.165,33	1.529.280,93	1.561.136,82	1.583.504,57	1.599.637,13
CH4 Combustion in CO2e	3.685,17	2.779,78	1.739,90	1.056,15	
CH4 Ventilation in CO2e	32.395,13	25.073,04	16.663,50	11.133,47	
CO2 Combustion in CO2e	3.547,78	3.516,30	3.478,44	3.457,59	
CO2 Ventilation in CO2e	487,53	486,78	485,91	485,34	

Figure 10. *Table generated by the iThink Software showing the total CO2e and partial CO_2 and CH_4 emissions from combustion and ventilation. over the 30 years of the simulation.*

3.4. Results Obtained

The main objective of the model is to meet the recommendations of "Subpart W" of Regulation 40 CFR Part 98 of the USEPA [19], which although valid for companies operating in the North American oil basins, its requirements are perfectly applicable to the Brazilian market. The USEPA requirements are relevant in that they require that emission inventories inform not only their total volumes in CO_2e, but also the emissions broken down by GHG and type of source. The development of the model layout allows the USEPA requirements to be met, but presents more detailed information, as it allows the estimation of emissions from each specific source, throughout the evaluation period. In view of this, the model can present the following estimates:

1. Sector 1: total CH_4 emissions from ventilation, converted to CO_2e;
2. Sector 2: total CH_4 emissions from combustion, converted to CO_2e;
3. Sector 3: total CO_2 emissions from ventilation, converted to CO_2e;
4. Sector 4: total CO_2 emissions from combustion, converted to CO_2e;
5. Sectors 1 + 2: total CH_4 emissions, converted to CO_2e;
6. Sectors 3 + 4: total CO_2 emissions, converted to CO_2e;
7. Sectors 1 + 3: total emissions from ventilation, converted to CO_2e;
8. Sectors 2 + 4: total emissions from combustion, converted to CO_2e;
9. Total emissions of each source group, in metric tons of their GHG;
10. Total emissions of each specific source in metric tons of its GHG;

11. Total emissions of the installation converted to CO_2e.

Once the model was assembled in order to meet the requirements of "Subpart W", the simulation was generated and resulted in the presentation of several important pieces of information. The main one is the generation of the information required by "Subpart W", synthesized by the table represented by Figure 10, extracted from the Control Panel. Figure 11 reproduces in an integral form the same table presented in Figure 10, corresponding to the accumulated volumes of CO_2e along the 30 years of simulation, as well as the annual volumes of CO_2 and CH_4 emission in CO_2e, discriminated between the combustion and ventilation sources, also in CO_2e. These data serve as the basis for the graph presented in Figure 12. In summary, all information generated by the model can be presented in tabular or graphical form, facilitating the necessary analyses.

10:10 03/07/2023 Table 2 (Total CO2e and partial CO2 and CH4 emissions from combustion and ventilation.)

Years	Total CO2e	CH4 Combustion in CO2e	CH4 Ventilation in CO2e	CO2 Combustion in CO2e	CO2 Ventilation in CO2e
1,00	0,00	0,00	15.263,85	0,00	485,76
2,00	15.749,62	0,00	38.663,21	0,00	488,18
3,00	54.901,00	0,00	69.755,53	0,00	491,38
4,00	125.147,92	0,00	84.982,92	0,00	492,95
5,00	210.623,78	0,00	84.251,17	0,00	492,88
6,00	295.367,83	0,00	78.029,25	0,00	492,24
7,00	373.889,32	0,00	64.064,71	0,00	490,80
8,00	438.444,83	0,00	50.715,07	0,00	489,42
9,00	489.649,32	0,00	39.183,48	0,00	488,23
10,00	529.321,03	0,00	32.063,96	0,00	487,50
11,00	561.872,48	0,00	28.310,96	0,00	487,11
12,00	590.670,55	0,00	28.813,08	0,00	487,16
13,00	619.970,79	0,00	34.052,76	0,00	487,70
14,00	654.511,26	0,00	40.552,38	0,00	488,37
15,00	695.552,01	0,00	47.609,44	0,00	489,10
16,00	743.650,54	0,00	52.209,19	0,00	489,57
17,00	796.349,30	0,00	54.588,02	0,00	489,82
18,00	851.427,14	0,00	56.185,97	0,00	489,98
19,00	908.103,10	0,00	57.179,27	0,00	490,09
20,00	965.772,45	0,00	57.252,88	0,00	490,09
21,00	1.023.515,43	0,00	54.718,96	0,00	489,83
22,00	1.078.724,22	0,00	48.614,55	0,00	489,20
23,00	1.127.827,97	0,00	44.477,31	0,00	488,78
24,00	1.172.794,05	0,00	41.805,06	0,00	488,50
25,00	1.215.087,61	0,00	37.735,81	0,00	488,08
26,00	1.253.311,51	0,00	32.395,13	0,00	487,53
27,00	1.286.194,17	0,00	25.073,04	0,00	486,78
28,00	1.311.753,98	0,00	16.663,50	0,00	485,91
29,00	1.328.903,39	0,00	11.133,47	0,00	485,34
Final	1.340.522,20				

Figure 11. *Table generated by the iThink Software showing the volumes of emissions calculated by the model, referring to accumulated Emissions in CO_2e, and broken down by type of source and type of GHG.*

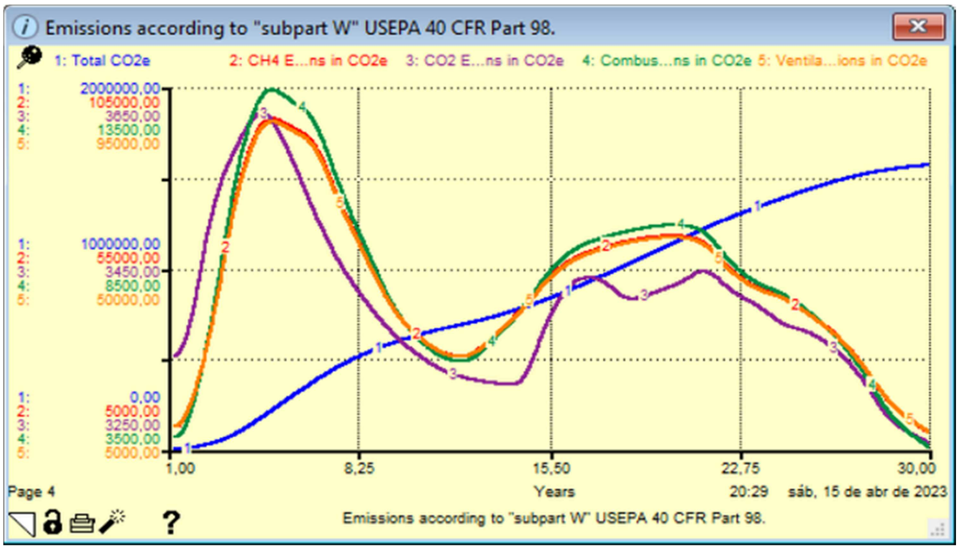

Figure 12. *Graphical representation of the information available in the Table shown in Figure 11.*

Various other information can be obtained, such as comparative curves of GHG emission profiles generated by the inclusion or exclusion of sources or source groups (Figure 13), emission profiles of specific sources (Figures 14 and 15), emission profiles of source groups and GHG type (Figure 16), among many others at the modeler's discretion, which characterizes the model's broad flexibility.

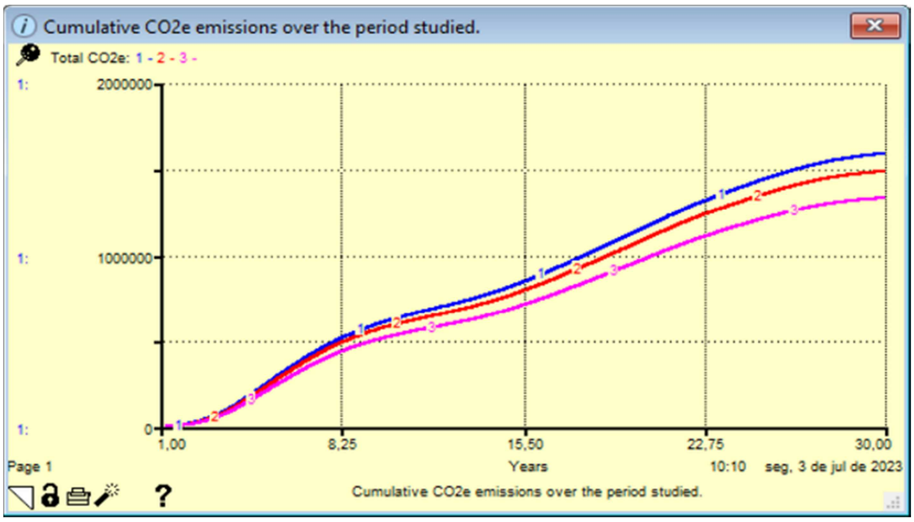

Figure 13. *Cumulative comparative emissions of* CO_2e.

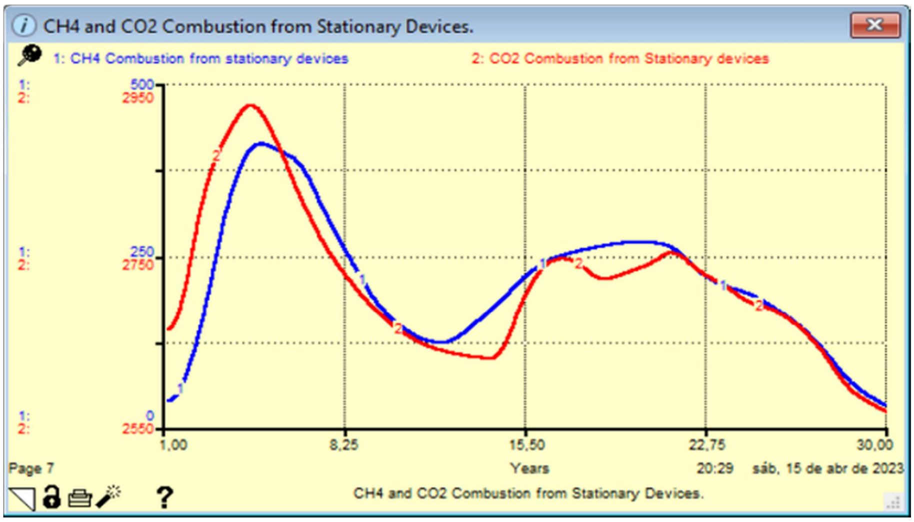

Figure 14. CH_4 *and* CO_2 *emissions from Stationary Devices.*

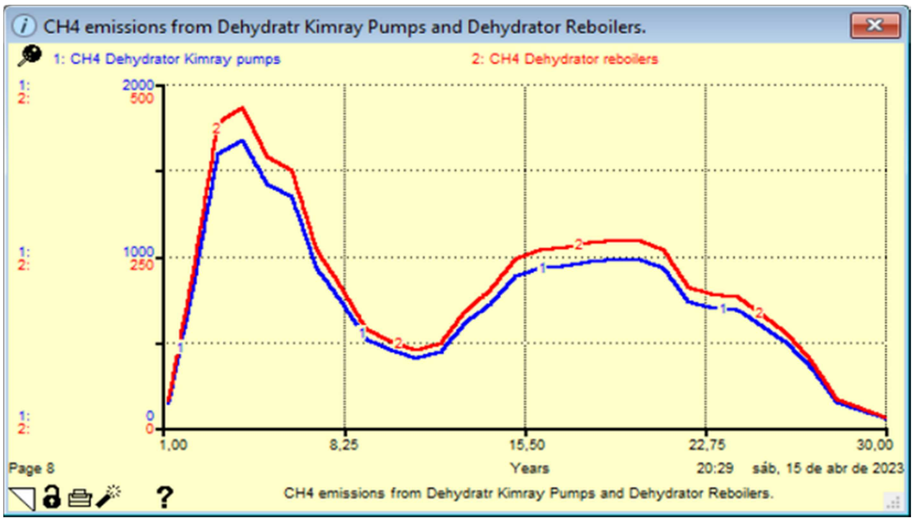

Figure 15. CH_4 *emissions from Dehydratr Kimray Pumps and Dehydrator Reboilers.*

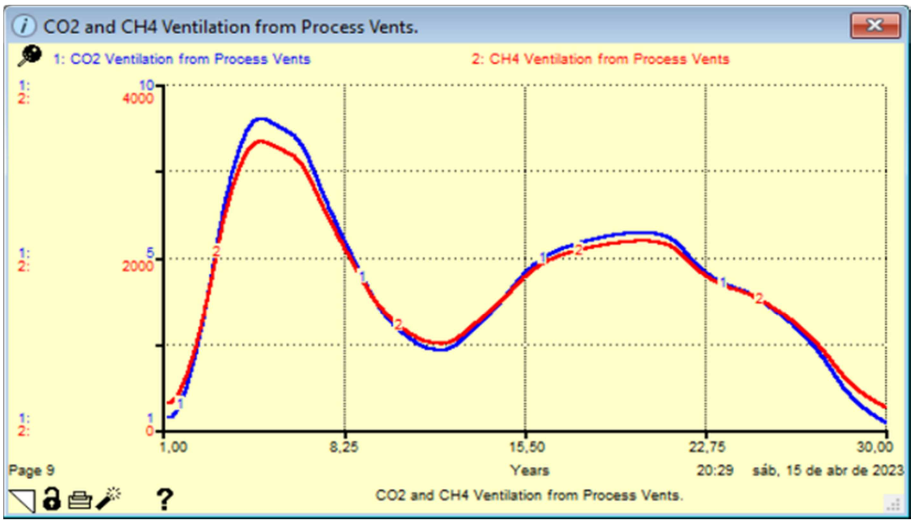

Figure 16. *Itemized emissions of CO_2 and CH_4 from Process Vents.*

Each of the graphs shown in Figures 13 to 16 can have their values tabulated as in Figure 13. This information provides the modeler with a complete set of information that enables him to determine which actions to take in order to mitigate emissions and at which points of the facility such actions should be taken. This clearly defined view of the behavior of emissions over the simulated period, their distribution by source type, by specific sources or groups of sources, and by gas type allows for vastly improved decision-making capabilities in generating or changing policies in order to mitigate emissions. This is just one example that demonstrates the power of the information generated by the proposed model.

There are two interesting aspects to be highlighted in the model. On the one hand, the model presented here is not limited to meeting the requirements of "Subpart W" of the USEPA CFR Part 98 Regulation. Its dynamic behavior allows not only estimating GHG emissions at a given moment in time, but goes beyond, allowing following the expected behavior of emissions throughout the simulation period. This characteristic allows the operator of the facility whose emissions are being modeled to plan ahead for maintenance or process changes, in order to meet internal requirements or environmental regulations that limit emissions. On the other hand, the model was developed in such a way that each specific emission source can be connected or disconnected from the set of emissions. This feature allows a wide range of estimates to be made, from the emissions of a single specific source, through the total emissions of groups of sources, emissions of each gas, and of course, to the total emissions. The combined effect of these two characteristics gives the model great flexibility, allowing the modeler to manipulate specific variables or sets of variables according to their operational objectives or compliance with environmental regulations.

4. Conclusions

The use of System Dynamics in the modeling of atmospheric emissions inventories of Greenhouse Gases (GHG) proves to be an important tool for the preparation of emissions inventories, since its ability to manipulate each variable separately or in groups generates numerous distinct output information, which allows the quantification of emissions from each specific source, identifying the importance of each variable or set of variables. Thus, considering each source of GHG emissions as a variable, the definition of the relevance of each source in the overall emissions calculation allows for the directing of attention and resources on the specific points of the most relevant oil and gas exploration and production facilities in terms of emissions.

The presented model, just based on CO_2 and CH_4 emissions, allows the generation of relevant informations, to the point of allowing the implantation of management policies and maintenance of facilities that effectively contribute to the reduction of emissions. However, at any time, at the discretion of the modeler and the needs of the entrepreneur, the inclusion of other emission sources and N_2O can be done, simply by redesigning the model including such information.

Therefore, considering the high costs that any changes in oil facilities can represent for companies, the use of System Dynamics for modeling air emissions in the oil and gas E&P area proves to be a powerful tool for analysis, planning, and cost control.

An important change that should be evaluated and possibly incorporated into the model is the inclusion of hydrocarbon stoichiometry as an auxiliary variable. The chemical composition of hydrocarbons is extremely variable, so that if we take into consideration that the Emission Factors available in literature are based on average carbon content of commercial hydrocarbons, standard conditions of temperature and pressure and specifications of calorific content, we see that the sources of error are extensive and tend to aggregate. Therefore, the use of data specific to the hydrocarbons exploited by the facility being modeled will already be a great advance towards minimizing uncertainties.

Once the re-evaluation of the current stage and concluded a new and more embracing version of the model is developed, its use will allow the inventories to cease to be mere accounting tools and to become effective environmental management tools, allowing the compatibility between emission reductions and viability in terms of costs.

Acknowledgements

This article is dedicated to the memory of Professor Isaac José Antonio Luquetti dos Santos, from the Federal University of Rio de Janeiro, whose scientific excellence, friendship, and mentoring are greatly missed by all those who lived with him.

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