Theoretical Calculations on Simultaneous Emission Removal from a Waste Gasification Plant

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Abstract:- This study presents a detailed and comprehensive methodology for theoretical engineering calculations in a modelled waste gasification plant. The aim is to determine the most effective way to clean up exhaust gases or emissions from industrial combustion processes. The pollution from chemical processes is significant due to the direct emission of harmful gases into the atmosphere, such as SO_x , NO_x , CO_x , O_3 , etc. To achieve this, we utilised the ASPEN PLUS simulation computer program, which facilitated a series of theoretical calculations during the procedure and optimisation of capturing the abovementioned dangerous gases and cleaning them out. This work involves two processes: the absorption of chimney's emissions from waste gasification plants, which consists mainly of a reactor and an absorber, and cleaning the contaminated remaining liquid from the absorber at the end of the capturing process. Through meticulous simulation and computer calculations, we have determined the absorbing rate of the polluting gases and completed a thorough sensitivity analysis for the entire process. This precision in our calculations instils confidence in our results' reliability and the proposed methods' potential effectiveness, reaffirming the trust in our research findings.

Key-Words: environmental pollution, pollutant gases, gas oxides, simulation, absorbing solutions, emission reduction.

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1. Introduction

1.1. The process of capturing acidic oxides consists of a reaction that makes oxidation possible, followed by a cooler that cools the oxidised gases. This mixer combines the NaOH solution and an 'absorption column '. This column is a critical component that allows the oxidised gases to be absorbed, a crucial step in the emission reduction process.

In the procedure below, the currents represent the following: 1: the stream of ClO₂ 2: the stream of polluting gases (NO, NO₂, SO₂, SO₃, etc.); 3- streams of oxidised gases 4- streams of cold water 5-flow of cold oxidised gases 6-flow of water and NaOH; 7-stream leaving the mixer and containing the cold NaOH solution; 8-the stream of steam that is released from the absorber must contain as few polluting gases as possible; 9-the solution

stream that leaves the reactor and includes all the salts formed [1-3].

1.2. The process of the Acidic gases Captured from the combustion processes

the process diagram Through flowsheet preliminarily constructed by us (see Figs. 1 and 2), the capture of all the harmful gases that come out of the chimneys of burning plants is realised before releasing them into the atmosphere. In stream 1, we have a mixture of gases where, in addition to sulfur and nitrogen oxides, we also have other 'polluting gases', a term used to describe the gases that contribute to environmental pollution [4–7].

The reactor used in this case is of the CSTR type, a crucial component that enables the oxidation of these gases by forming the corresponding salts of each pollutant. In stream 2, we have ClO2, which is used as an oxidiser. In-stream three, we have oxidised gases, which pass to a scrubber or an absorber, where water absorption becomes possible [8–9].



Schematic presentation of the CSTR reactor followed by an absorber in the simulation software ASPEN PLUS.

Here, we have the separation of condensable gases from non-condensable gases. Condensable gases stay in the water and form 'polluting water', a byproduct that requires further treatment. At the fig. 2 it is presented a tentative process diagram of acidic gases capture, where non-condensable gases are released into the atmosphere because they are harmless—the capture of combustion gases. Through this scheme, we capture all the gases that come out of the chimneys of plants or factories as secondary material so as not to release them directly into the atmosphere. Stream 1 has a mixture of sulfur, nitrogen oxides, and other polluting gases [11].



Fig. 2: Acidic gases capture process diagram using EdrawMax software

In stream 2, we have ClO2, which is used as an oxidiser. In stream 3, we have oxidised gases, which then pass to a scrubber or an absorber where absorption by water becomes possible [10].

Fig. 3 Schematic presentation of the CSTR



absorber in the simulation software ASPEN PLUS.

Here, we have the separation of condensable gases from non-condensable gases. Condensable gases stay in water and form polluting water, while non-condensable gases are released into the atmosphere because they are harmless.

1.3.Capture of combustion gases.

Through this scheme, all the gases that come out of the chimneys of plants or factories as secondary material make it possible to capture them so as not to release them directly into the atmosphere. In stream 1, we have a mixture of gases where, in addition to sulfur and nitrogen oxides, we also have other polluting. The reactor used in this case is of the CSTR type, which makes it possible to oxidise these gases by forming the corresponding salts of each pollutant. In stream 2, we have ClO_2 [12], which is used as an oxidiser. In-stream three, we have oxidised gases, which then pass to a scrubber or an absorber where absorption by water becomes possible. Here, we separate condensable gases from non-condensable gases, which stay in water and form polluting water. In contrast, noncondensable gases are released into the atmosphere because they are harmless [13-15].

The general scheme worked on Aspen Plus is formulated as in the flow sheeting of Fig 4.

2. Material and Methods



Fig. 4: Full absorption process diagram of SO_x and NO_x gases with solution ClO2 in ASPEN PLUS V11.

The modelling and simulation of technological processes were conducted using a standard methodology. This approach, widely accepted in the field, involves determining and optimising process indicators and engineering capacities. The physicochemical properties used in the simulation were taken from the built-in databases of the ASPEN PLUS software, ensuring the results' accuracy and reliability.

For many scientific problems, especially technological development, the data for the dynamic construction of technological processes does not exist. However, they are sufficient for the so-called stationary (steady-state) models. Because of this, the time dependencies of all influencing parameters cannot be considered, which is why the modelling and related calculations become much more straightforward. The simulation/modelling scheme represents technological plants' construction, development, and operation. Depending on the desired details, we are dealing with fundamental technological schemes, piping schemes, and instruments. The simulation scheme graphically presents a process, showing the basic operations for the various parts of the plant, which are connected through material and energy flows. By calculating the mass and energy balances, it is possible to calculate the mass and ratios of productive currents, such as pressure and temperature. Regarding the principle that through design and modelling programs are carried out calculations, we distinguish sequential modular calculations of basic operations according to their arrangement in the process diagram (flowsheet) and simultaneous calculation of all stages through the passage of all elements in the equalisation system.

Sequential modular calculation of individual essential elements has some advantages in modelling, as it performs comprehensible simulations, detects errors, and offers the possibility of adding models. Comparing it with simultaneous calculations, we found some areas for improvement in the case of opposite currents and recycling between basic operations since they have to be repeated many times. Let us consider the flow control for the flowsheet simulation performed throughout the computer program. Through it, the models for calculating the functions were obtained one after the other, basically mutually related to the data of subjects, mixtures, or thermodynamic models. Other numerical subroutines were used to solve linear and non-linear equations encountered in separate modules.

It is important to describe some of the essential technological parts of operation by the chemical reaction equations used while modelling various technology processes for producing synthetic fuels, together with their symbols.

3. Results and Discussion

Specifications for raw materials: In this work, the raw materials are polluting gases and an oxidiser that converts gases with a low oxidation number into gases with the highest oxidation number. We have raw NOx, SOx, CO2, O2, ClO2, and H2O raw materials as in table 1.

Components	Content	Density	Molar
(kg/m^3)		(kg/m^3)	mass
			(kg/kmol)
NO _x	200	1.34	27
	ppm		
SO_2	65 ppm	2.93	64
O ₂	9 %	1.43	32
CO ₂	13 %	1.98	44
air	79%	1.29	

Table 1 Some specific properties of the gases

Reactor feedstock: Gas flow: Polluting gases are collected from all the chimneys of plants, factories, or anywhere there is a combustion reaction and the release of gases.

We have summarised the input data for the raw material in the following table, which presents the input current flows, the percentages of each current component, the temperature of the input components, and their pressure (see Table 2).

Values on this table has been taken from the laboratory experimental characterisation for the

actual situation taken into account for this research.

Table 2: Typical exhaust gas compositions

Components	NOx, ppm	SO ₂ ppm	O ₂ ,%	CO ₂ ,%	Humid, ity %	Air
Waste- burning treatment plant	200	65	9	13	0	78%
Conversion in %	0,02	0,0065	9	13	0	78

The input currents in this table are in ppm or %, but in the Aspen Plus program, we have replaced the unit kg/sec as the total flow as well as the content of the components in the current. Rapid Tables software was used for unit conversion, which made it possible to convert ppm to percentages, knowing the density of each component and converting these percentages to the program unit km/hr. First, we find the total flow in km/hr and mp after each component (see Table 3).

 Table 3: Summary of component input measures

Components	Kg/s
NO	9.5
SO ₂	6.06
O ₂	6.217
CO ₂	6.17
Air	72.056

The input currents in this table are in ppm or %, but in the Aspen Plus program, we have replaced the unit kg/sec with the total flow and the content of the components in the current.

Reactor specifications: The reactor used in the process is of the CSTR type; its function is the oxidation of gases. Some summary data for the reactor

Specifications	Streams	Kine	tics ØPSE	Component	Attr.	Utility	Catalyst	Comment
Operating condition	ons							
Pressure			1	atm	•			
Temperature			453	к				
O Duty				Watt	- 4			
Vapor fraction								
Valid phases Specification type	Vapor-O Reactor	nly volume			•	2nd	Liquid	
Reactor			Pha	;e				-
Volume	20	mi	 Phase 	ie 🖉				
volume	30	sec	- Volu	me		cum		
Resi, time			1000					
Resi, time			Volu	metrac				

Fig. 5: Reactor completions in Aspen Plus V11

All reactions are kinetic and have their constants, the release or acquisition of energy.

New	Edit Co	ppy Paste	
Rxn No.	Reaction type	Stoichiometry	Delete
1	Kinetic	NO + CLO2> NO2(MIXED) + CLO(MIXED)	×
2	Kinetic	NO + CLO> NO2(MIXED) + CL(MIXED)	×
3	Kinetic	CL + CLO2> 2 CLO(MIXED)	×
4	Kinetic	NO + NO2> N2O3(MIXED)	×
5	Kinetic	2 NO2> N2O4(MIXED)	×
6	Kinetic	N2O4> 2 NO2(MIXED)	×
7	Kinetic	SO2 + CLO> SO3(MIXED) + CL(MIXED)	×
8	Kinetic	2 CL> CL2(MIXED)	×
9	Kinetic	2 CLO> CLO2(MIXED) + CL(MIXED)	×

Fig. 6: Reactions entered in Aspen Plus V11

The feedstock of the reactor are the following components: the stream of ClO_2 and the stream of

polluting gases (NO, NO₂, SO₂, SO₃, etc.). A packed tower is chosen as the absorbing device. The packed towers are filled with packing





Tests in Aspen Plus: Our work in Aspen Plus has been multiple, and each has an addition or subtraction of the process. Evidence number 1: In the program, I entered all the devices and all the currents as shown in the theory above, but I could not find a method that included NaOH; the simulation went to the end, but the results were not very satisfactory and expected.

The process calculation in the first trial consisted of a CSTR reactor, a cooler, a mixer and an absorber. The input streams in the process were polluted gases, chlorine oxide, cold water in the cooler, water needed to form the NaOH solution, and the NaOH stream entering the mixer. The completion seen in the figure above is done for all other reactions.

The program entered all the devices and all the currents, as shown in the theory above, but I needed help finding a method that included NaOH. The simulation went to the end, but the results could have been more satisfactory. The process in the first trial consisted of a CSTR reactor, a cooler, a mixer and an absorber.

The input streams in the process were polluted gases, chlorine oxide, cold water in the cooler, water needed to form the NaOH solution, and the NaOH stream entering the mixer. The completion

seen in the figure above is done for all other reactions.



Fig. 8: Test number 1 in Aspen Plus Test number 2

In test #2, We tried to dump the NaOH stream from the mixer since it was not generated using our method in Aspen Plus.

The process continued to generate results at the end, but again, they did not obey our theory of releasing as little gas as possible at the end. Again, the process had the same equipment and initial data in all currents and equipment specifications.



Fig. 9: Test number 2 in Aspen Plus

The following figure shows this process:

Test number 3

In test number 3, seeing that the mixer was not playing an important role but only mixing water with the temperature coming out of the cooler with water coming from normal conditions and seeing that their temperature was close to their temperature in out of the mixer, we thought we'd remove one and see what the results would be like in the end. The simulation again ran to completion, and some data was generated, but we still needed to meet our expectations. The figure below shows the process where the mixer is missing.



Fig. 10: Test number 3 in Aspen Plus

Test number 4

In this test, we added another device at the end of the process where we have the solution output containing the dissolved gas salts. Suppose these crypts get out into the environment. In that case, they can be harmful to the environment, and to eliminate this occurrence, we have added another absorption column where it is possible to absorb these salts. The figure below represents this simulation:

Test number 5:



Fig. 11: Test number 4 in Aspen Plus

In this test, it was added a second cooler and made it possible to reduce the surface area of the cooler by dividing it into two equal parts, that is, since in the summary table of the supplement for the cooler, we have an area of 1248 m2 by dividing it into two equal parts for both exchangers is 624m2.

In Fig. 11, S1 represents the water entering the cooler, S2 the exit of cold gas oxides, S3 the exit of warm water from the first cooler (B1), S4 the NaOH solution that enters the mixer (B2), S5 the union of the three streams of water at the same temperature, S6 water under normal conditions enters the second cooler (B3), S7 warm water from the second cooler, S8 cold oxides, S9 current where we have the reduction of polluting gases, S10 salt solution exit.

Test number 6: We have considered only SO_x reactions in this test, assuming these gases are present only in the stream. The only difference is that we have considered only the reactions that occur for SOx, eliminating all other pollutants.

Test number 7: In this test, we only considered NO_x , eliminating all other pollutants that may be present in the flue gas stream. So, in the reactor, we have the kinetic reactions of NO_x being oxidised and then absorbed to prevent their release directly into the atmosphere.

Although the most critical tests were mentioned above, many other tests in Aspen are related to changes in some parameters of currents or devices.

Materia	Heat Load Work Vol% Carves	Wit % Curves Pa	Anthern Polyme	n Salida							
		Units	c1.02 -	64Z •	OXVGAZ .	\$1 .	2 .	ş	59 -	\$10 -	
	Phase		Vapor Phase	Vapor Phase	Vapor Phase	Liquid Prase	Vapor Phase	Liquid Phase	Vapor Phese	Liquid Phase	
	Temperature	£	298	298	453	288	293.15	291.561	329,239	268.858	
	Pressure	Ni/sqm	101325	101325	101325	101325	101325	101325	101325	101325	
	Molar Vapor Fraction		3	1	1	0	1	a.	1	0	
	Molar Liquid Fraction		Ū.	0	0	1	ņ	1	e	1	
	Molar Solid Fraction		0	0	0	0	ġ	a	0	0	
	Mass Vapor Fraction		Ť.	i. if	1	0	. T	0	1	0	
	Mass Liquid Fraction		0	0	0	1	- 0	31	. 0	£.	
	Mass Solid Fraction		D	Q.	0	0	0	G	0	0	
	Molar Entitalpy	Ukriol	1.02402++08	-2.67438e+07	-1.8862e+07	-2.86591e+08	-2.37457e+07	-2.86322#+08	-4.05527e+07	-2.84737e+08	
	Mass Enthelpy	ing	1.51815e+06	-859442	-589408	-1.59082e+07	-742047	-1.58933e+07	-1.45414e+06	-1.55921e+07	
	Molar Entropy	Jikmei-K	-59916.6	5245.95	17403.5	+165822	4119.96	-164897	2859.55	-164250	
	Mass Entropy	Jäg-K	-888.291	168.585	543,831	-9204.51	128.742	-9153.16	102.26	-8994.27	
	Molar Density	kmol/cum	0.0414705	0.0409299	0.0269031	\$5,4664	0.0416166	55,4332	0.0370553	\$3,1473	
	Mass Density	kg/cum	2.79725	1.27364	0.860943	999.243	1.3318	998.645	1.03619	970.555	
	Enthelpy Row	Watt	151815	-1.58997e+06	+1.14935e+06	-3.18164e+08	+1.44699e+06	-3.17866e+08	-2.36291e+06	-3.1691e+00	
	Average NW		67.4515	31.1176	32:0016	18,0153	32,0016	18,0153	27.9634	18.2616	
1.4	Mole Hows	kmol/sec	0.00148255	0.0594519	0.0609344	1.11017	0.0609344	1.11017	0.0581101	1.11299	
1	Mole Fractions										
100	• Mass Flows	kg/sec	0.1	1.85	1.95	20	1.95	20	1.62495	20.325	
10	Mass Exactions										
	Volume Bow	cum/sec	0.0357494	1,45253	2.26496	0.0200151	1.45418	0.0200271	1.5682	0.0209417	
	Vapor Phase										
12	Liquid Phase										

Some results and graphs generated by Aspen Plus

Fig. 12: Results when using reactions for SO_x only

Mat	terial Hast Load Vol.% Curves Wt.	% Curves Petroleum	Polymen Soli	da:		
		Units	CLO2 -	GAZ +	OXYGAZ -	-
	Cost Flow	\$/sec				
F	- MIXED Substream					
•	Phase		Vapor Phase	Vapor Phase	Vapor Phase	
Þ.	Temperature	к	298	298	453	
P	Pressure	N/sqm	101325	101325	101325	
6.	Motar Vapor Fraction		1	1	1	
8	Molar Liquid Fraction		a	0	0	
P.	Molar Solid Fraction		0	o	0	
b.	Mass Vapor Fraction		1	1	1	
þ.	Mass Liquid Fraction		0	o	0	
P.	Mass Solid Fraction		0	0	0	
£-	Molar Enthalpy	J/kmol	1.02402e+08	-1.20249e+08	-2.61121e+07	
E.	Mass Enthalpy	J/kg	1.51815e+06	+2.73467e+06	-490481	
h.	Molar Entropy	J/kmol-K	-59916.6	-6424.91	-5084.49	
K)	Mass Entropy	J/kg-K	-888.291	-146.114	-95.5052	
н.	Molar Density	kmol/cum	0.0414705	0.0411169	0.0269692	
9	Mass Density	kg/cum	2.79725	1,80799	1,43578	
8	Enthalpy Flow	Watt	1.51815e+06	-2.73467e+06	-980962	
F.	Average MW		67.4515	43.9719	53.2379	
6	+ Mole Flows	kmol/sec	0.0148255	0.0227418	0.0375673	
Þ.	Mole Fractions					
9×	Mass Flows	kg/sec	1	1	2	
R.	+ Mass Fractions		-			
1	Volume Flow	cum/sec	0.357494	0.553101	1.39297	

Fig. 13: Numerical calculations results for the reactor

81 (Heat3) - Stream Results (Boundary) = [1	84 Column Internets IF(T-1)	B4.Currfiguratio	PEAKTOR (RCSTRJ-Setup =	Bid Column Internals INT-1 Ser	tions
Mat	terral Float Lunal Vol.76 Curves V	P. S. Curves Petroleuro	Padyment Sola	44.			
		Drifts	52 -	37 -	59 -	510 -	-
- 1	Cost Flow	\$/eec	(b)				
	- MOCED Substream						
	Phase		Vapor Phase	Liquid Phase	Vapor Phase	Liquid Phase	
	Temperature	K	292.15	290,899	329.994	299.713	
	Pressure	Nilegm	101325	101325	101325	101325	
	Molar Vapor Fractices		(1	0	1	0	
	Molar Ciguid Fraction		0		0.		
4.1	Motar Solid Fraction		0	0	0	0	
	Main Vapor Fraction		1	.0	7	0	
	Mess Liquid Fraction		0		0		
b -1	Mass Solid Fraction		0	0	0	0	
	Motar Enthalpy	3/Kencel	-3:25638e+07	-2.06372e+08	-2.44945e+07	-2.70601#+08	
	Mass Enthalpy	1/kg	-611067	-1.58961e+07	-802363	-1.43512a+U7	
+	Molar Entropy	I/formed+K	-22975.7	-165068	1133.7	-160154	
	Mass Entropy	J/hig-K	-424.054	-9162.64	37,0711	-8364.87	
	Molet Density	kmpl/cum	0.0419351	55.44	0.0169685	53.1504	
10	Maue Demoity	kg/cum	2.23234	998.767	1.12857	1017.63	
*	Enthalpy Flow	Watt	-1.22553e+06	-8.17921e+08	-52232.7	-3.19166e-DB	
	Average MW		\$3,2279	18.0152	10.528	19.1462	
	+ Mole Flows	kmol/eec	0.0375673	1.11017	0.00213243	1.1456	
	+ Mole Fractions						
	+ Mass Flows	kg/sec	2	20	0.0650987	21.934	
	* Mass Fractions		100				
	Volume Flow	SWITV/ARS	0.095842	0.0200247	0.0576832	0.021554	

Fig.14: Results for the absorber

The following charts, 1-4, show the dependence of mass and the number of plates in the column, the dependence of mass on plates in different phases, the dependence of temperature on plates, and the dependence of temperature in the cooler, respectively.



Chart 1: Mass and number of plates in the column



Graph 2: Dependence of mass on plates in different phases



Graph 3: Dependence of temperature on plates



Graph 4: Dependence of temperature in the cooler

4. Conclusions and Recommendations

In anticipation of the calculated results that the Aspen Plus program should have generated, it should be within the expectations described in the theory above. The NO_x and SO_x gases at the outlet of the gas vapour stream at the outlet of the absorber should have been sufficiently reduced about the measures we have set at the inlet. Input measures were taken from the literature, and some reports and component measures were found from the reactions. In conclusion, the polluting gas should have been reduced so that after oxidation with chlorine oxide and interaction with different bases, they could form more salts dissolved in water than components released in the gas vapours from the absorber.

If the stream of gases released above the reactor has more pollutants than the stream below the reactor, then we have something that could have been done better with the program, or that needs to be added to our data. If the stream of salt solutions has a large amount of pollution, it will not be a problem since we can add a treatment plant for these waters and make them harmless to the environment.

Our interest is only in the one at the outlet of the absorber gases, and there, we have to minimise the components of NO_x and SO_x as much as possible.

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