



Research article

Nitric oxide recovery from hydrogen combustion streams. A clean pathway for the sustainable production of nitrogen compounds

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ARTICLE INFO

Keywords:

Sustainability
Gas absorption
Nitric acid production
Thermodynamic modeling
Hydrogen combustion

ABSTRACT

This work proves that nitric oxide (NO) can be successfully recovered from hydrogen flue gas streams in nitric acid, opening new pathways for NO control in combustion streams. Recovering NO from hydrogen combustion streams allows for increasing the combustion temperature in the turbine, reducing the fuel consumption per kWh, while obtaining a building block for nitric acid production. The solubility of nitric oxide is determined in amines, ethanol, and nitric acid solutions at a laboratory scale, suitable candidates for nitric oxide absorption. The solubility of nitric oxide in amines and ethanol is very low (0.009 mol/L/bar & 0.018 mol/L/bar respectively) compared with nitric acid (0.23 mol/L/bar), which is in the same range as the solubility of CO₂ in amines solutions. Nitric acid, in addition to having good NO solubility, also presents high selectivity towards nitric oxide and easy recovery of nitric oxide by simply raising the temperature. Finally, a fugacity-activity coefficient model combining the Peng-Robinson (PR) equation of state with the Non-Random Two-Liquid (NRTL) activity coefficient model is proposed as a thermodynamic model to represent the NO-HNO₃-H₂O equilibrium, giving as a result an average absolute deviation between the experimental results and the model predictions of only 5%.

1. Introduction

One of the main drivers of the current energy transition is the decarbonization of the energy production system by replacing fossil fuels with cleaner alternatives, such as wind and solar-based technologies (IEA, 2024; Okere and Sheng, 2023). However, because of the high variability in renewable energy production (low sunshine and low wind days), there is a growing interest in developing technologies that can efficiently store the surplus of electricity when the renewable electricity production capacity exceeds the electrical demand. In this context, one of the most promising technologies is green hydrogen production and storage, where the extra energy produced by solar or wind sources during low-demand periods is used to power an electrolyzer to produce hydrogen, which can be stored and subsequently converted into electricity during periods of low renewable energy production capacity and high electrical demand (Egeland-Eriksen et al., 2021). Being aware of the high potential of green hydrogen as an energy vector due to its high energy content (Okere and Sheng, 2024), governments have created programs and strategies to promote the development of a green hydrogen infrastructure and a green hydrogen market. In the case of the

European Union, the ambition is to produce 10 million tons and import 10 million tons of renewable hydrogen by 2030 (European Commission, 2022).

To foster research on hydrogen conversion into electricity, the European Union is currently allocating funds to projects that aim to expand the use of the existing combined-cycle power plant by installing gas turbines capable of using hydrogen as a fuel (European Commission, 2020). Although hydrogen combustion is CO₂-free (Onorati et al., 2022), the main drawback is the high amount of NO_x (mainly composed of nitric oxide) generated during combustion, being three times larger than in the case of natural gas due to the higher adiabatic flame temperature of hydrogen (Cappelletti and Martelli, 2017). Even though nitric oxide (NO) is not a greenhouse gas, it is still a serious pollutant, as it is the main precursor of smog and acid rain (Lasek and Lajnert, 2022). Nowadays, the most common method to control NO emissions in hydrogen combustion processes is to reduce the temperature in the gas turbine, as this parameter is directly related to NO formation. Although this is an effective measure in terms of NO emissions control, it reduces the thermodynamic efficiency of the turbine (Nemitalah et al., 2018). Alternative NO control technologies are available for fuel gas and

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<https://doi.org/10.1016/j.jenvman.2024.122561>

Received 25 May 2024; Received in revised form 29 August 2024; Accepted 16 September 2024

Available online 20 September 2024

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natural gas combustion, including selective catalytic reduction and three-way catalysts. These technologies present some disadvantages such as problems with the high water vapor content in the flue gas, high operational/capital costs, and some disposal problems (Gholami et al., 2020) that penalize their implementation in hydrogen combustion at an industrial level. Moreover, these technologies are based on the reduction of NO molecules to N₂, preventing the use of NO as a building block for other nitrogen-based processes.

In this paper, a new technique for NO control based on gas absorption is presented. The fundamentals are basically the same as those of the industrial-scale existing technologies for CO₂ and H₂S emissions control based on gas absorption (Mandal and Bandyopadhyay, 2006). Although some authors have already studied the solubility of nitric oxide in some solvents, a suitable candidate has not been found yet. Khan and Adewuyi (2010) studied the NO absorption in sodium persulfate solutions finding that the absorption was based on the interaction of NO with hydroxyl ions (OH⁻) and sulfate ions. They achieved absorption yields of up to 92% with 0.1M of sodium persulfate. However, to reach this yield, the reaction had to maintain a pH above 9, requiring constant addition of basic solutions, generating high operating costs. The same authors studied NO absorption by a combination of persulfate and ferrous-EDTA obtaining almost 100% removal with a mixture of 0.1M persulfate with 0.01M Fe(II) and 0.01M EDTA (Adewuyi and Khan, 2015). As in the previous study, the absorption rate was strongly dependent on the pH and the oxygen concentration, being difficult to control in a flue gas stream. Fine and Rochelle (2014) analyzed the absorption of a NO and NO₂ mixture on monoethanolamine (MEA), piperazine (PZ), and methyldiethanolamine (MDEA) achieving NO₂ absorption rates of 99%. Nonetheless, 15% of the absorbed NO_x was converted into nitrosamines, toxic and carcinogenic compounds (Magee, 1971) and no NO absorption yield was reported in the article. None of the authors mentioned above described the possibility of recovering NO by desorption, as in all the scenarios NO was intended to be eliminated rather than recovered. Carta and Pigford (1983) studied the NO absorption in nitric acid solutions of concentrations varying between 10 and 35% w/w at 25 °C and 1 atm, aiming to determine a NO mass transfer model. The experimental part of this work showed that the use of a nitric acid solution with a concentration between 25 and 30% w/w increased the absorption rate. On the other hand, the theoretical part of this work revealed that although the penetration theory can be used to explain the NO absorption rates in nitric acid, it does not account for equilibrium limitations. The article did not present data about NO solubility in nitric acid nor of the impact of temperature and pressure in the process. Finally, Hughes (2008), Deng and Deitrich (2007) and Michalski et al. (2022) studied the reaction of NO with different alcohols, as this system has a high relevance in physiological systems. They determined that this reaction proceeds via NO reduction, producing nitroxyl or alkyl nitrate. Nonetheless, no data of NO solubility in ethanol was reported.

The main challenge for NO absorption is to find a suitable absorbent that can overcome the low solubility of NO in conventional solvents (Khan and Adewuyi, 2010), having a high selectivity towards NO in the flue gases, and allowing NO desorption without any degradation. Finding a suitable absorbent for nitric oxide recovery will not only improve the hydrogen combustion process by reducing the fuel consumption per kWh of electricity produced, but it will also allow for obtaining nitric oxide, which can be used as a building block in the production of nitrogen-based derivatives such as nitric acid (HNO₃). Nitric acid is obtained by the oxidation of ammonia to nitric oxide and then to nitric dioxide, which is hydrated to nitric acid (Ostwald process), and currently accounts for 80% of the ammonium nitrate used in the production of fertilizers. Ammonia is currently produced by the Haber-Bosch process, a technology that consumes approximately 2% of the world's energy and is responsible for 1.8% of global CO₂ emissions (Ojelade et al., 2023). The use of nitric oxide recovered from the hydrogen combustion stream in nitric acid production could lead to a

drastic decrease in CO₂ emissions, which are expected to achieve 200 MtCO₂/yr in 2050 (Lim et al., 2021).

After reviewing the existing literature on nitric oxide absorption, three promising candidates, tested in this work, have been found.

1. Amines: NO₂ and NO absorption occur via the formation of nitrosamines, nitrites, or nitrates in the same ranges of temperature and pressure as the absorption of CO₂ and H₂S in amines (Fine et al., 2014; Fine and Rochelle, 2014). The current utilization of these absorption technologies at an industrial scale (Mandal and Bandyopadhyay, 2006) can speed up the deployment of a NO-amines-based absorption process. Three amines were tested: aminomethyl propanol (AMP), methyldiethanolamine (MDEA), and triethanolamine (TEOA). Some authors (Fine and Rochelle, 2014; Zhao et al., 2007) have studied nitric oxide and nitrogen dioxide absorption in amines, but no experimental data has been reported for pure nitric oxide.
2. Ethanol: although ethanol is not currently used at an industrial scale for the absorption of polluting compounds of flue gas streams, apart from being a widely available and relatively non-expensive solvent, ethanol is expected to have a higher NO solubility than amine compounds because of the chemical reaction between NO and ethanol (Suarez et al., 2015). Moreover, ethanol has been also used in other existing nitric oxide post-combustion techniques such as in selective catalytic reduction (Miyadera, 1997).
3. Nitric acid solutions: The reaction between nitric oxide and nitric acid has been studied in the context of the Ostwald process (nitric acid production). However, no experimental data on nitric oxide solubility at different temperatures and pressures is available. These studies are mainly focused on reducing the amount of nitrous acid produced (Isupova and Ivanova, 2019) in the process. The NO absorption rate and solubility are expected to be higher in nitric acid than in amines or ethanol because of the dissociation of nitric acid into nitrate (NO₃⁻), a radical that reacts with nitric oxide. Furthermore, nitric acid is a commodity and, at the same time, a nitric oxide derivative.

To briefly summarize the results of this work, a nitric oxide solubility of 0.04 mol/L (AMP) was obtained for the tested amines, 0.08 mol/L for ethanol, and 1.25 mol/L for nitric acid. The optimal solvent for NO absorption was found to be a 30% v/v solution of nitric acid, having the highest solubility, being a selective solvent towards NO, and allowing for NO recovery by desorption.

2. Materials and methods

2.1. Materials

Aminomethyl propanol C₄H₁₁NO - AMP (95%) and methyldiethanolamine C₅H₁₃NO₂ - MDEA (99%) used in the experiments were purchased from Sigma. Nitric acid- HNO₃ (65%) and triethanolamine C₆H₁₅NO₃ - TEOA (99%) were purchased from Panreac and Ethanol C₆H₆O (99.9%) from Davila Villalobos. Type 1 Mili-Q water was used for the preparation of the reactants. Nitric oxide - NO (99.5%) was purchased from Linde.

2.2. Experimental setup

The experimental setup presented in Fig. 1 was used to measure the solubility of nitric oxide in different liquids. The setup consists of a 29 ml absorption vessel where 15 ml of the absorbent liquid is placed. The liquid is stirred constantly at 130 RPM using an IKA RCT classic magnetic stirrer, except during the loading of nitric oxide. NO is introduced into the reactor from a 2 m³ B10 bottle using a pressure reducer (PI1) to control the inlet pressure, and a SITEC needle valve, leak-tested for 24 h with nitrogen, to regulate the flow. The pressure change inside the absorption vessel is monitored by a Druck dpi 104 digital pressure gauge

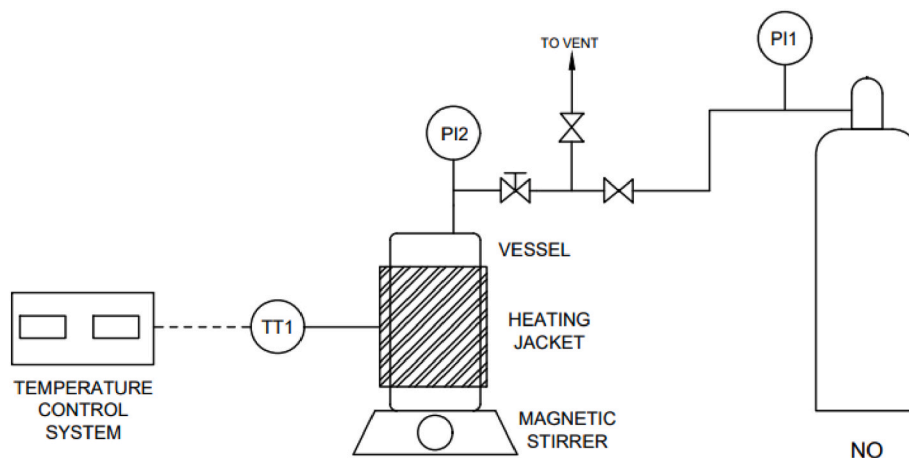


Fig. 1. Nitric oxide absorption. Experimental setup.

(PI2). The temperature control system consists of an Axiomatic BS-2100 PID controller which allows monitoring and adjusting the temperature inside the absorption vessel. Rock wool is used to avoid heat loss. The equipment has a ventilation system to evacuate the nitric oxide safely after the end of the experiment. Piping, fittings, and the absorption vessel are made of stainless steel to prevent corrosion.

2.3. Procedure

The experiment is conducted in a closed vessel where equilibrium is reached and starts by placing 15 ml of the absorbent liquid in the absorption vessel. The liquid is degassed by a combination of freezing with liquid nitrogen and vacuum (up to 0.02 bar) to evacuate all the gas from inside the vessel. The vessel is then heated to 35 °C to release the gases dissolved in the absorbent liquid. The process is repeated at least 2 times until the pressure inside of the reactor, after heating, is less than 0.05 bar. Once degassed, the absorption vessel is connected to the temperature control system, and stirring is started. Heating is initiated by selecting the desired temperature on the temperature control system. Once the temperature remains constant, the initial pressure, which belongs to the partial pressure of the absorbent liquid at the selected temperature, is recorded. The absorption vessel is pressurized by adjusting the pressure-reducing valves (PI1) and slowly opening the needle valve. While NO is charged, stirring is stopped to minimize the NO absorption. The pressure is monitored for approximately 2 h and when there is no further pressure decrease for at least 30 min, equilibrium is assumed to have been reached.

The solubility of nitric oxide in the absorbent liquid is calculated by the pressure decay method, in which the difference between the initial pressure (P_i) and the final pressure (P_f) (equilibrium pressure) determines the number of moles of nitric oxide dissolved in the absorbent liquid:

$$n_{NO} = \frac{V^*(P_f - P_i)}{T^*R^*Z} \quad \text{Equation 1}$$

where V is the gas volume in the vessel, T is the temperature in K, R is the gas constant, and Z is the nitric oxide compressibility factor, which is calculated based on the data reported by Goldin and Sage, with values close to 1 for all the experimental conditions (Golding and Sage, 1951). After each experiment, the final liquid volume was measured, verifying a negligible change with respect to the initial volume value. Once a desired equilibrium pressure is reached, the reactor is pressurized further (maintaining the temperature) to reach the next equilibrium pressure. Duplicates were made for each absorbent liquid.

3. Results and discussion

Nitric oxide absorption was tested on amines, which are industrially used for CO₂ and H₂S absorption, ethanol, which is widely available and used in other NO control technologies (Miyadera, 1997), and nitric acid, which is a nitric oxide derivative.

According to the literature, the concentration of NO in flue gases from hydrogen turbines varies between 500 and 8000 ppm (Chiesa et al., 2005; Kroniger et al., 2017; Luo et al., 2019; Shadidi et al., 2021) being the main compounds water, nitrogen, and nitric oxide (Ditaranto et al., 2015). However, pure NO was tested in this work since water vapor is expected to condensate before the absorption tower and the solubility of nitrogen in the absorbent liquids tested in this work is very low (Fine and Rochelle, 2014; Grande et al., 2018; Saliba et al., 2001). In the flue gas stream, a small amount of N₂O or NO₂ could be found in the case of an oxygen-rich operation (Shchepakina et al., 2023). Their presence is expected to have a minor influence on the process since N₂O will be decomposed by hydrogen radicals (Colorado et al., 2017) and NO₂ will be easily solubilized in the condensed water before the absorption column (Jarvis et al., 2010).

The temperatures selected to evaluate the NO solubility in all the absorbent liquids vary between 35 and 65 °C, as these are the typical operating temperatures of other industrial absorption processes such as CO₂ or H₂S absorption in amines (Bernhardsen and Knuutila, 2017). In industrial applications, the outlet temperature of CO₂ in the flue gases is typically around 1200 °C and decreases to 150 °C in a secondary steam turbine. Then, the flue gases are either released through the stack (Song et al., 2004) or sent to a CO₂ absorption process which typically operates in a range of 30–60 °C (Rochelle, 2009). The temperature range evaluated in this article (35–65 °C) is in line with existing absorption technologies for pollutant control. The pressures evaluated are between 1 and 7 bar following the typical pressure values used for H₂S and CO₂ industrial absorption processes (Shoukat et al., 2019; Stewart, 2014).

3.1. Amines

The removal of CO₂ and H₂S by amine absorption is a well-known process established on an industrial scale (Mandal and Bandyopadhyay, 2006). Absorbing nitric oxide in amines could leverage existing CO₂ and H₂S absorption technologies. Although only a few articles present some results on nitric oxide absorption by amines, it is known that primary amines react with NO₂ and NO to form unstable nitrosamines that are decomposed into a carbocation and nitrogen, secondary amines form stable nitrosamines (Fine et al., 2014), and tertiary amines form nitrates and nitrites (Fine and Rochelle, 2014). Since nitrosamines are highly toxic compounds (Magee, 1971) it is not recommended to use

secondary amines as absorbents (Rochelle et al., 2001). Thus, only primary and tertiary amines were tested. Although it is known that nitrosamines do not revert to nitric oxide (Fine and Rochelle, 2014), these experiments aimed to determine the extent to which amines could solubilize nitric oxide.

The solubility of nitric oxide in the primary amine aminomethyl propanol (AMP) and the tertiary amines methyldiethanolamine (MDEA) and triethanolamine (TEOA) was tested at 1, 3, 5, and 7 bar, 35 °C and 40% w/w amine concentration. The results for the NO absorption in the three tested amines are shown in Fig. 2 and more detailed in the Supplementary Materials (Table S1). At 1 bar most of the amines have similar solubility values between 0.0055 and 0.0070 mol/L. After 3 bar a break occurs, and AMP starts having higher values than MDEA and TEOA. Finally, at 7 bar, AMP shows the highest solubility (0.0445 mol/L). Compared with the solubility of CO₂ in monoethanolamine (0.58 mol/L/bar) (Wagner et al., 2013), amines do not seem to be a promising candidate for nitric oxide absorption. The explanation of the low solubility of nitric oxide in amines is given by Hughes (2008). Nitric oxide is a stable radical that does not react easily with other molecules that are not radicals. Amines are organic compounds that do not present any radicals in their structure, therefore the reaction that occurs between NO and amines is not easily promoted, being even independent of the amine concentration (Hughes, 2008; Smith and Loepky, 1967). To accelerate the reaction rate, a small presence of air or a catalyst is required (Williams, 1983).

3.2. Ethanol

Nitric oxide absorption in ethanol is expected to proceed at a higher absorption rate and yielding higher solubilities than in the case of amine absorption because of the possibility of producing, as reaction compounds, alkyl nitrite or nitroxyl (Equation (2)) (Deng and Deitrich, 2007; Suarez et al., 2015). Thus, the solubility of nitric oxide in ethanol was tested at 1, 3, 5, and 7 bar and 35 °C. Fig. 3 and Table S1 (Supplementary Materials) present the results for the nitric oxide solubility in ethanol, showing a solubility twice as high (0.082 mol/L) as that obtained for the best case with amines (AMP 0.048 mol/L). Even though there was an improvement in the NO solubility, this value is still far away from the solubility value for CO₂-MEA (0.58 mol/L/bar), showing that ethanol is not a suitable alternative for NO absorption on an industrial scale.

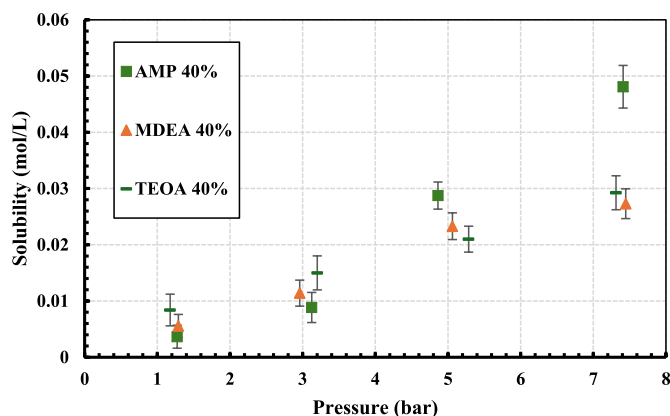
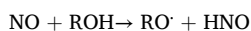


Fig. 2. Experimental data of NO solubility in three types of amines (AMP 40%, MDEA 40%, and TEOA 40%) as a function of pressure (between 1 and 7 bar) at 35 °C.

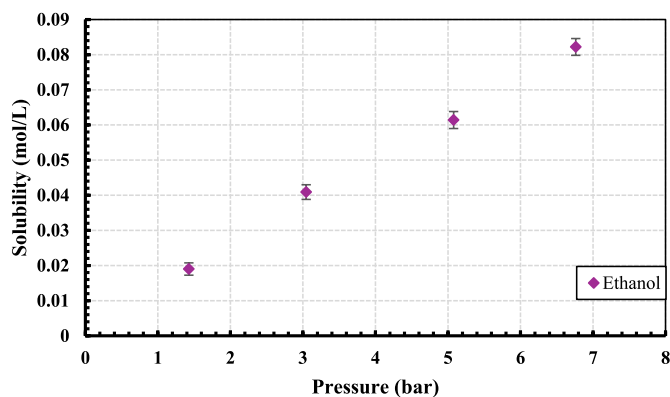
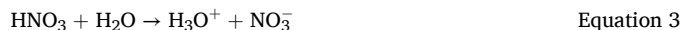


Fig. 3. Experimental data of NO solubility in ethanol as a function of pressure (between 1 and 7 bar) at 35 °C.

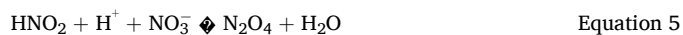
3.3. Nitric acid

The last set of experimental studies aimed to analyze the solubility of nitric oxide in nitric acid (HNO₃) solutions. Nitric acid is a commodity produced from nitric oxide in the well-known Ostwald process. The absorption of nitric oxide in nitric acid has been previously studied by some authors such as Carta and Pigford (1983), who reported the absorption rate and kinetics of nitric oxide absorption in nitric acid solutions up to 35 wt%, 25 °C, and 0.3–1.0 atm. Additionally, Lefers (1980) studied the oxidation and absorption of nitric oxide in nitric acid, focusing on the oxidation conditions of nitric oxide using 63–78 wt% nitric acid solutions, and determining in which phase the reaction happened. Finally, Weisweiler et al. (1991) studied the kinetics of NO absorption at 30–60 wt% nitric acid solutions, 25 °C, 1 bar, and NO concentration from 250 to 10,000 ppm, focusing mainly on NO mass transfer. Although all these works analyzed the absorption of NO in nitric acid, they did not provide solubility values in the temperature and pressure ranges presented in this work. To our knowledge, this work is the first to analyze the variation of NO solubility in a temperature and pressure range suitable for the design of a post-combustion absorption process for NO recovery.

Compared to nitric oxide absorption in amines and ethanol, the dissociation of nitric acid in water yields a nitrate radical (NO₃[•]) as a product (Abel and Schmid, 1928), a radical compound that reacts with nitric oxide improving the absorption rate and the solubility:



The solubility of nitric oxide in nitric acid solutions proceeds according to the equilibrium reaction shown in Equation (4) (Carta and Pigford, 1983; Counce, 1977; Lefers, 1980), further detailed by Abel (Equation (5) and Equation (6)) (Abel and Schmid, 1928). The main advantage of nitric acid over other absorbent liquids is the fact that, after nitric oxide absorption, the formed nitrous acid (HNO₂) will decompose back into nitric oxide and nitric acid just by raising the temperature, allowing the recovery of nitric oxide.



According to Lefers (1980), the reaction presented in Equation (4) for nitric acid concentrations between 78 and 63% v/v takes place mainly in the gas phase due to the considerable vapor pressure of nitric acid. At nitric acid concentrations between 63 and 40% v/v, it occurs partially in the gas phase and partially in the liquid phase. Finally, at nitric acid concentrations below 40% v/v, the reaction occurs entirely in the liquid phase with only nitrous acid (HNO₂) as the final product.

Therefore, to avoid vaporization, the experimental conditions selected in this work considered nitric acid solutions at 10, 20, 30, and 40% v/v concentrations, 1 bar of equilibrium pressure, and 35, 45, 55, and 65 °C of equilibrium temperatures. Nitric acid decomposition is not expected to occur under the evaluated conditions because of the inhibitory effect of water in the operating conditions tested in this work (Robertson, 1954). Moreover, the absorbent volume was measured before and after each experiment, showing minimum volatilization of nitric acid (volume difference always lower than 1%).

The highest solubility (Table S2, Supplementary Materials) was obtained for a 30% v/v nitric acid solution for the whole temperature range, as shown in Fig. 4. The difference in the solubilities obtained for 30% and 40% v/v solutions is not remarkable, but the slight decrease for a 40% v/v nitric acid solution could correspond to some partial vaporization of nitric acid. The results at 1 bar agree well with those obtained by Carta and Pigford (1983) who studied the absorption rate of nitric oxide in aqueous nitric acid solutions at concentrations up to 35% v/v. These authors found that nitric oxide absorption was catalyzed by high concentrations of HNO_2 , obtaining the highest absorption rate ($5 \text{ mol/s} \cdot 10^5$) in a 35% v/v nitric acid solution. According to Counce (1977) and Chacuk et al. (2007), higher nitrous acid concentrations are not beneficial, since, when operating with nitric acid concentrations higher than 40% v/v, the produced nitrous acid decomposes again back to nitric acid and nitric oxide (Equation (4)). Based on the above-mentioned results, a 30% v/v nitric acid concentration solution was selected as the optimal absorption solution, as it yields the highest NO solubility, and the reaction proceeds in the liquid phase obtaining a stable product (HNO_2), allowing better control of the overall process.

The solubility of nitric oxide in a 30% v/v nitric acid solution was further evaluated at 1, 2, 3, 4, 5, and 6 bar and 35, 45, 55, and 65 °C. Higher pressures were not tested since the flue gas stream containing nitric oxide is expected to come from the exhaust of a hydrogen turbine (Chiesa et al., 2005). The results of this evaluation are presented in Fig. 5 and Table S3 (Supplementary Data). As expected, the highest solubilities were obtained at the minimum temperature (35 °C) and the maximum pressure (6 bar). The highest solubility (0.23 mol/L/bar) was obtained at 35 °C and 30% HNO_3 , being in the same range as the solubility of CO_2 in MEA (0.58 mol/L/bar) (Wagner et al., 2013). This figure proves the high potential for the industrial implementation of this technology, thanks to the existing similarities with the widespread technologies for H_2S and CO_2 recovery by gas absorption (Asghar et al., 2021). Lower investment and complexity are expected for this technology in comparison with the current NO control technologies (Zhao et al., 2021). Moreover, this technology could be also applied to nitric oxide control in

ammonia combustion streams. The feasibility of the process should be further analyzed by studying the variation in the concentration of the different species (NO , NO_2 , N_2O , NH_3 , O_2), at different operating conditions.

Comparing the results of this work, the highest solubilities were obtained in nitric acid solutions (0.27 mol/L, 30% v/v solution at 35 °C and 1 bar), followed by ethanol (0.02 mol/L at 35 °C and 1 bar), and then, the amines compounds (0.008 mol/L, 40% TEO amine solution at 35 °C and 1 bar). This is explained by the fact that, while nitric oxide is chemically absorbed in nitric acid and ethanol (Carta and Pigford, 1983; Hughes, 2008), in the case of the amines compounds there is no reaction with nitric oxide because of the low nitrosating capacity of this compound (Williams, 1983). Comparing the absorption processes in ethanol and nitric acid, while ethanol reacts with nitric oxide via a reduction reaction producing nitroxyl, an unstable molecule (Shafirovich and Lymar, 2002), nitric acid is dissociated into a nitrate radical (NO_3^-) which easily reacts with nitric oxide via a radical-radical reaction yielding nitrous acid, a more stable compound (Carta and Pigford, 1983).

Based on the results of this work, nitric acid is selected as the optimum nitric oxide solvent as it yields the highest solubility, is less volatile than ethanol, and does not generate toxic byproducts, such as in the case of the amines.

4. Thermodynamic modeling

The high solubility of nitric oxide in nitric acid is a clear opportunity to consider the design of absorption equipment to recover this contaminant from a flue gas stream. To be able to address the engineering calculations required in the design of such pieces of equipment, a proper thermodynamic model, able to accurately fit experimental solubility data, needs to be available (Suleman et al., 2015). For this reason, we present in this section a new equilibrium model for the $\text{NO-HNO}_3\text{-H}_2\text{O}$ system, that can be used in the design of absorption equipment. To our knowledge, this is the first time that a thermodynamic model precise enough to describe the NO solubility in nitric acid has been reported. Because of the lack of data on NO solubility in nitric acid at different temperatures and pressures, for the validation of the thermodynamic model, only the experimental data obtained in this work have been used.

The equilibrium model is based on the classical fugacity-activity coefficient approach ($\phi - \gamma$). In this work, the Peng-Robinson-Boston-Mathias Equation of State (PRBM EoS) together with the Non-Random-Two-Liquid activity coefficient model (NRTL) were selected

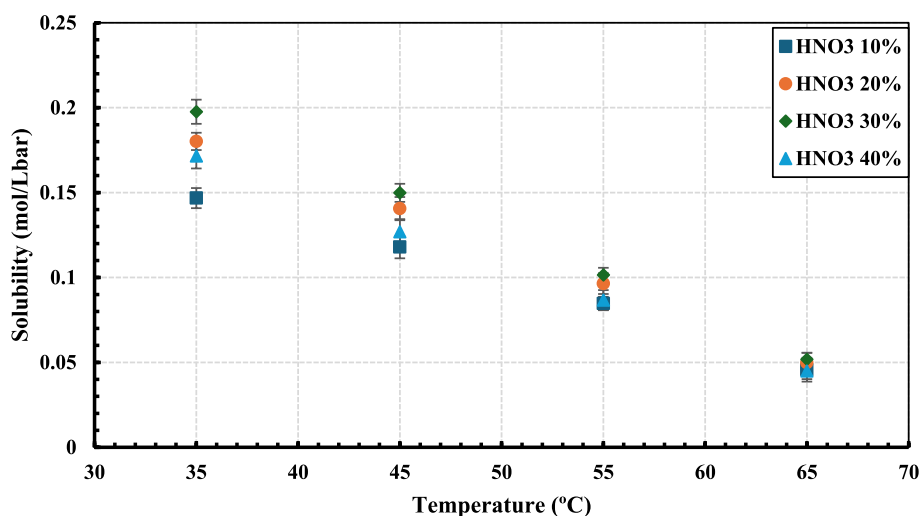


Fig. 4. Experimental data of NO solubility in HNO_3 solutions at different concentrations (10, 20, 30, and 40% v/v) as a function of temperature (between 35 and 65 °C) at 1 bar.

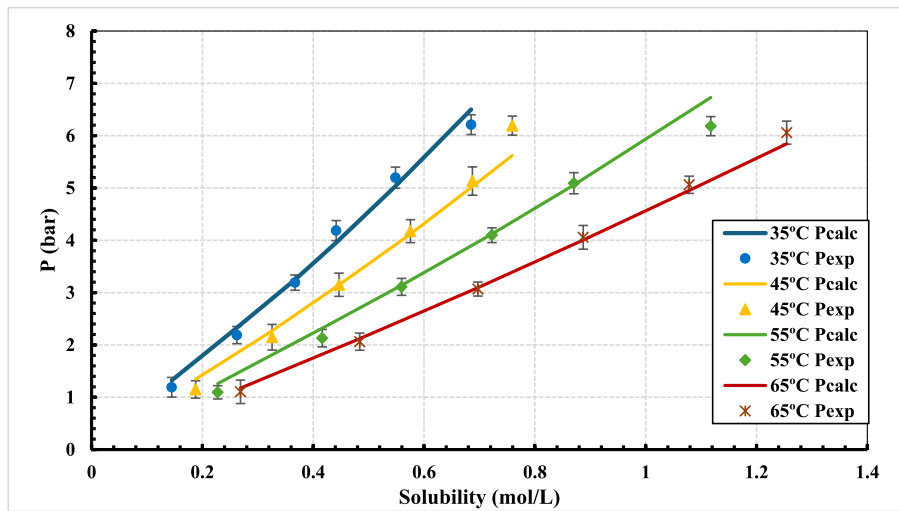


Fig. 5. NO solubility in a 30% v/v HNO₃ solution as a function of pressure (between 1 and 6 bar) at temperature conditions between 35 and 65 °C. Comparison between experimental measurements (points) and model prediction (continuous lines).

because of the polarity of water and nitric acid, and because even though the pressures are not very high, it provides more precise results than only considering the ideal approach for the vapor phase. The equilibrium equations (Equation (7), Equation (8), and Equation (9)) can be expressed as:

$$\phi_{NO} \cdot P \cdot y_{NO} = \gamma_{NO} \cdot H_{NO} \cdot x_{NO} \quad \text{Equation 7}$$

$$\phi_{HNO_3} \cdot P \cdot y_{HNO_3} = \gamma_{HNO_3} \cdot P_{HNO_3}^s \cdot x_{HNO_3} \quad \text{Equation 8}$$

$$\phi_{H_2O} \cdot P \cdot y_{H_2O} = \gamma_{H_2O} \cdot P_{H_2O}^s \cdot x_{H_2O} \quad \text{Equation 9}$$

Where ϕ is the vapor phase fugacity coefficient, γ is the liquid phase activity coefficient, P is the total pressure, y is the vapor phase molar fraction of each component, x is the liquid phase molar fraction of each component, $P_{HNO_3}^s$ (Equation (10)) and $P_{H_2O}^s$ (Equation (11)) are the saturation pressure of nitric acid and water at the equilibrium temperature, and H_{NO} is the Henry's constant of NO in the nitric acid solution. The partial pressures of nitric acid (Equation (10), (Duisman and Stern, 1969)) and water (Equation (11) (Posey and Rochelle, 1997)) were also taken into consideration by including their corresponding equilibrium equations. This is especially relevant for nitric acid, with a higher volatility than water (Pradhan et al., 1997):

$$P_{HNO_3}^s = \frac{10^{7.61628 - \frac{1486.238}{T(^{\circ}C) + 230}}}{750.062} \quad (\text{bar}) \quad \text{Equation 10}$$

$$\ln P_{H_2O}^s = 72.55 - \frac{7206.7}{T} - 7.1385 \cdot \ln T + 4.046 \cdot 10^{-6} \cdot T^2 \quad (\text{Pa}) \quad \text{Equation 11}$$

The vapor phase fugacity coefficients are calculated using the Peng-Robinson equation of state (Equation (12)) (Peng and Robinson, 1976) together with the modified Boston-Mathias alpha function (Boston and Mathias, 1980), which is useful to represent the behavior of a gas at temperatures above the critical temperature, as in the case of nitric oxide (Equation (13)–(15)).

$$\ln \frac{\phi_i}{x_i P} = \frac{b_i}{b} (Z_c - 1) - \ln(Z_c - B) - \frac{A}{2\sqrt{2}B} \left(\frac{2\sum_j X_j a_{ji}}{a} - \frac{b_k}{b} \right) \cdot \ln \left(\frac{Z_c + (1 + \sqrt{2}B)}{Z_c - (1 - \sqrt{2}B)} \right) \quad \text{Equation 12}$$

$$\alpha(T, \omega) = \left\{ \exp \left[c \cdot (1 - T_r^d) \right] \right\}^2 \quad \text{Equation 13}$$

$$d = 1 + m(\omega)/2 \quad \text{Equation 14}$$

$$c = 1 - d \quad \text{Equation 15}$$

The mixture parameters a (Equation (16)) and b (Equation (17)), of the Peng-Robinson equation of state are defined by the one-parameter van der Waals mixing rules. These mixing rules were chosen as they are simpler than other mixing rules (two parameters van der Waals, Huron-Vidal, Wong-Sandler), but with similar precision on the result.

$$a = \sum_i \sum_j x_i x_j a_{ij} \quad \text{Equation 16}$$

$$b = \sum_i x_i b_i \quad \text{Equation 17}$$

$$a_{ij} = (1 - k_{ij}) \cdot \sqrt{a_i^* a_j} \quad \text{Equation 18}$$

In the case of the NRTL model, the non-random parameter χ_{ij} was assumed to be equal to 0.3 for the NO-HNO₃-H₂O system, as it fits in the Type I category proposed by Renon and Prausnitz (1968). Equation (19) determines the binary interaction parameters (τ_{ij}).

$$\tau_{ij} = \frac{NRTL A_{ij} + NRTL B_{ij}}{T} \quad \text{Equation 19}$$

While the values of the NRTL parameters for the HNO₃-H₂O system were available in the Aspen Plus® Database (APV120 ENRTL-RK, Table 1) and the values of the NRTL parameters for H₂O-NO and NO-H₂O were set to zero due to the low interaction expected between these molecules (Hughes, 2008), the values of the NRTL parameters for the NO-HNO₃ system, considered symmetrical, were obtained by non-linear regression.

Finally, the Henry constant was defined by Equation (20) (NIST, 2023), where p and q are unknown parameters determined by non-linear regression:

Table 1
NRTL model parameters. HNO₃-NO & HNO₃-NO parameters were obtained by non-linear regression. HNO₃-H₂O & H₂O-HNO₃ parameters were taken from Aspen Plus® (APV120 ENRTL-RK database).

	HNO ₃ -NO	NO-HNO ₃	HNO ₃ -H ₂ O	H ₂ O-HNO ₃	NO-H ₂ O	H ₂ O-NO
NRTL _A	-19.852	-19.852	0	0	0	0
NRTL _B	4735.3	4735.3	3259.3	-710.9	0	0

$$H_{NO} = \frac{1}{p^* e^{q^* \left(\frac{1}{T} - \frac{1}{298.15} \right)}} \text{ (bar)} \quad \text{Equation 20}$$

The values of the NRTL parameters for the NO-HNO₃ system (Table 1) and the Henry equation coefficients p (0.0067) and q (2020.5), were obtained by non-linear regression (*lsqcurvefit* Matlab function), minimizing the difference between the experimental equilibrium pressure and the equilibrium pressure calculated by the model.

The average absolute deviation (AAD%), selected to determine the accuracy of the model is defined as:

$$AAD\% = \frac{1}{n} \sum_{i=1}^n \left(\frac{p^{calc} - p^{exp}}{p^{calc}} \right) \cdot 100 \quad \text{Equation 21}$$

Where p^{calc} is the total equilibrium pressure calculated by the model and p^{exp} is the experimental equilibrium pressure.

The model provides an excellent fitting of the experimental results (Fig. 5, Table S3) with an AAD% of only 5%. The high precision of the model allows for its consideration in the calculation of absorption equipment.

5. Conclusions

Nitric oxide recovery from hydrogen combustion streams is an opportunity for the cleaner production of nitrogen compounds such as nitric acid while improving the efficiency of hydrogen turbines. This work has determined the solubility of nitric oxide in three potential solvents for NO absorption: amines, ethanol, and nitric acid, in concentration, temperature, and pressure ranges suitable for the design of a post-combustion absorption-based process. Additionally, for the first time a thermodynamic model accurate enough (%AAD<5%) to represent the solubility of nitric oxide in nitric acid, the optimum solvent, is presented. The key findings of this work are presented below.

- The absorption of nitric oxide in amine solutions proceeds via the formation of nitrosamines, nitrites, or nitrates. Nitric oxide solubility in amines is penalized by the fact nitric oxide presents a low nitrosating capacity. The resulting solubilities are in the range of 0.009 mol/L/bar, being too low to be considered at an industrial scale.
- In the case of ethanol, the nitric oxide solubility is slightly higher than in amine solutions (0.018 mol/L/bar) as it is promoted by the formation of nitroxyl. However, it is still low to be considered at an industrial scale.

Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.jenvman.2024.122561>.

Nomenclature

Abbreviations	
NO	Nitric oxide
HNO ₃	Nitric acid
H ₂ O	Water
CO ₂	Carbon Dioxide
N ₂	Nitrogen
H ₂ S	Hydrogen sulfide
MEA	Monoethanolamine
AMP	Aminomethyl propanol
TEOA	Triethanolamine
MDEA	Methyldiethanolamine
EU	European Union
H ₂ SO ₄	Sulfuric acid
N ₂ O	Nitrous oxide
NH ₃	Ammonia

(continued on next page)

- Nitric oxide presents a very high solubility in nitric acid solutions (0.23 mol/L/bar), comparable to the solubility of CO₂ in amines (0.58 mol/L/bar for CO₂ in MEA) because of the reaction between nitric oxide and nitrate radicals formed by nitric acid dissociation. The reaction is favored by absorption temperatures and pressures in the same range as those used in current industrial absorption processes (CO₂-H₂S recovery). The fact that nitric acid is produced via oxidation and hydration of nitric oxide (Ostwald process) enables the direct integration between a nitric oxide absorption plant and a nitric acid production plant.
- The solubility of nitric oxide in nitric acid solutions can be successfully represented by a thermodynamic model based on the Peng-Robinson-Boston-Mathias Equation of State and the NRTL activity coefficient model. The average absolute deviation between the experimental results and the model predictions is only 5%.

The high solubility of nitric oxide in nitric acid solutions, the fact that after absorption, nitric oxide can be easily recovered by simply raising the temperature, and the high solubility towards nitric oxide, make nitric acid solutions an optimum candidate for the sustainable recovery of nitric oxide.

CRedit authorship contribution statement

Nataly Castro-Ferro: Writing – review & editing, Writing – original draft, Investigation. **Luis Vaquerizo:** Writing – review & editing, Writing – original draft, Validation, Supervision, Project administration, Methodology, Investigation, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

Acknowledgments

The authors thank the MCIN & FEDER for funding the project PID2022-140930NB-I00, and Castilla y León Regional Government & FEDER for funding the program CLU-2019-0).

(continued)

O_2	Oxygen
HNO_2	Nitrous acid
Symbols	
n_{NO}	Number of moles, component i (mol)
V	Gas volume in the vessel (L)
P_i	Initial experimental NO pressure (bar)
P_f	Final experimental NO pressure (bar)
T	Temperature (K)
R	Molar gas constant (0.08315 bar L/mol·K)
Z	Compressibility factor
ϕ_i	Vapor phase fugacity coefficient, component i
P	Pressure (bar)
y_i	Molar fraction of i component in the vapor phase
γ_i	liquid phase fugacity coefficient, component i
x_i	Molar fraction of i component in the liquid phase
H_{NO}	Henry constant of solubility of NO in 30% Nitric acid (bar)
$P_{H_2O}^s$	Saturation pressure of water at working temperature (bar)
$P_{HNO_3}^s$	Saturation pressure of nitric acid at working temperature (bar)
Z_c	Critical compressibility
A,B	Peng Robinson mixture parameters
a_i, a_j	Peng Robinson individual attraction parameter, component i,j
b_i	Van der Waals covolume, component i
$\alpha(T, \omega)$	Peng Robinson attractive function
ω	Pitzer's acentric factor
c	Boston-Mathias parameter c
d	Boston-Mathias parameter d
T_r	reduced temperature
a_{ij}	Peng Robinson combined attraction parameter, component i,j
k_{ij}	Peng Robinson binary interaction parameter, component i,j
τ_{ij}	NRTL binary interaction parameter
$NRTL_{A_{ij}}$	NRTL independent parameter
p,q	Henry constant of NO solubility parameters
p^{calc}	Calculated equilibrium pressure (bar)
p^{exp}	Experimental equilibrium pressure (bar)
So^{calc}	Calculated solubility (mol/L)
So^{calc}	Experimental solubility (mol/L)

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