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PhD Thesis:

ENERGY RECOVERY FROM INDUSTRIAL PROCESSES USING CHEMICAL SUBSTANCES

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PhD AIM

The aim of this research is to evaluate an innovative thermal VOCs abatement system, that also provide the energy valorization of raw waste wood from industrial processes. The energy consumption and the efficiency of a traditional system were analyzed, as well as the amount of raw waste produced by the case study company. These elements are used as a baseline data for a series of kinetic analysis using GasDs software. The simulations evaluate the simultaneous combustion of virgin waste wood biomass and air polluted by several solvents. Output data return the types of some reaction products, emitted in atmosphere, and the efficiency of VOCs abatement.

In the perspective of circularity and sustainable use of resources, this theoretical study, combined with the experimental data, aims to contribute at the reduction of the environmental impacts in terms of certain pollutant release and use of energy. This preliminary study can be, also, considered as a starting point for further research.

INTRODUCTION

The motivation behind this study should be find in everyday life. The air we breathe and the environment in which we live are unfortunately increasingly contaminated with pollutants. This condition is reflected in damage to human, animals, and ecosystems health; so clean air must be considered a basic requirement for healthy life and well-being.

The World Health Organization (WHO) estimates that environmental air pollution causes around 3.7 million deaths a year worldwide, 800,000 only in Europe. It is responsible for 6.3 million years of life lost and 3% of cardio-respiratory mortality. In a recent process of reviewing the scientific literature on the main pollutants, the WHO recommended to the European Union urgent policies for containing emissions and more stringent air quality standards (Health Organization & Office for Europe, 2013). By this Organization, air quality levels for 6 pollutants are recommended, where evidence has advanced the most on health effects from exposure. When action is taken on these "classical pollutants": Carbon Monoxide (CO), Sulphur Dioxide (SO_2), Nitrogen Dioxide (NO_2), Particulate Matter (PM) and Ozone (O_3), it also has an impact on other damaging pollutants (World Health Organization, 2000). Nowadays with industrial emissions optimization, energy saving, and green energy solutions will be possible to make a huge impact in reducing pollution and protecting the environment.

Pollution is defined as the introduction of substances harmful for humans and other living organism into the environment. These substances are possible solids, liquids, or gases produced in higher than usual concentrations that reduce the quality of our environment (Manisalidis et al., 2020).

Industries are one of the largest producers of pollutants, especially refineries, foundries, pesticide, chemical, plastic, wood, printing, painting, metal, and steel manufacturers.

In this research work, the woodworking sector was analyzed, with a focus on furniture and fixtures production from virgin raw material. Industries of this kind use a great amount of solvents for coating and generate a lot of virgin wood waste products.

The structure of this research thesis is composed by many parts:

- The sections 1 and 2 show the definitions of pollution and some pollutant compounds with a focus on the Volatile Organic Compounds management;
- The section 3 explains the type of emissions and background regulations to achieve the environmentally safe and quality targets;
- The section 4 describes the industrial abatement technologies and raw material waste management;
- The section 5 shows the case study factory;
- The section 6 proposes the innovative system evaluated as main research topic;
- The section 7 describes the experimental protocol used, composed by sampling campaigns and laboratory characterization;
- The section 8 consists in the theoretical phase, which involves the use of kinetic package for simulations;
- The section 9 explains the finding results;
- The section 10 shows the conclusions focused on the criticisms, their mitigations and the possible future research implications.

1. POLLUTION: VOCs, GhG AND PARTICULATE MATTER

Studies on the quality of human health have shown that one of the causes of premature death is environmental pollution. In fact, hundreds of millions of healthy life years are lost each year according to global air pollution assessments, particularly on individuals with chronic conditions, as well as older people, children, and pregnant women. Pulmonary insufficiency, chronic asthma, cardiovascular diseases, and cardiovascular mortality are some of the long-term effects associated with air pollution (Eze et al., 2014).

VOCs EMISSIONS

In recent decades, there has been an increased focus on air pollution and considerable efforts have been made on emission control and the reduction or elimination of polluting components, these include Volatile Organic Compounds (VOCs). These chemical species have many harmful properties to the health and environment (X. Zhang et al., 2021). For these reasons VOCs are listed in the group of the most undesirable air pollutants and need mitigation before releasing them in the environment. Especially in the working environment, the exposition to high concentrations of these compounds leads to the adverse impact on workers' health. In the Italian regulation, the Art. 298 of Legislative Decree N. 152/2006 ('Environmental Regulations') provides their definition. An organic component is any compound containing at least the element carbon (C) and one or more of the elements hydrogen (H), oxygen (O), fluorine (F), chlorine (Cl), bromine (Br), iodine (I), sulphur (S), phosphorus (P), silicon (Si) or nitrogen (N), with the exception of carbon oxides (e.g. CO2) and inorganic carbonates and bicarbonates. The same decree also gives the definition of a volatile organic compound: any organic component that has at 293.15 K (i.e. at 20 °C) a vapour pressure of 0.01 kPa or more, or that has a corresponding volatility under particular conditions of use (D.Lgs. n. 152, 2006).

The (Directive EU n. 42, 2004) defines a VOC as 'any organic compound having an initial boiling point of 250 °C or less, measured at a standard pressure of 101.3 kPa'. To this is added a subsequent subdivision by the World Health Organisation, which has identified four classes:

- very volatile organic compounds (VVOCs) that have a boiling point of < 0 to 50-100 °C;
- volatile organic compounds (VOC) that have a boiling point from 50-100 to 240-260 °C;
- semi-volatile organic compounds (SVOCs) that have a boiling point of 240-260 to 380-400 °C;
- particulate-associated organic compounds (POM) that have a boiling point above 380 °C.

VOCs can be divided into two categories according to their origin. They are:

- Biogenic VOCs, if the compounds are emitted in nature (e.g. terpenes);
- Anthropogenic VOCs, if the compounds are emitted by human activities (e.g. petroleum-derived solvents).

The main volatile organic compounds are listed below:

- *Aliphatic hydrocarbons* can be found in fuels, perfumes, propellants, refrigerants, paints, or insecticides. Propane, for example, is used as a fuel, as a refrigerant, as a solvent and as a propellant; butane is used as a fuel, as a refrigerant and as a reagent; hexane is used as a fuel and as a solvent.
- *Halogen derivatives* can be found in pesticides, degreasers, and refrigerants. Chloroform, for example, is used as a solvent, refrigerant, or glue; dichloromethane is used as a solvent.
- *Aromatic hydrocarbons* can be found in varnishes and paints, in glues, detergents and fuels. Benzene has been widely found in fuels, lubricants, paints, detergents

and to make other chemicals; toluene is used in fuels and as a solvent and reagent; xylene is used as a solvent, diluent and detergent.

- *Alcohols* can be found in detergents, disinfectants, paints, cosmetics, and adhesives. Ethanol is used as a solvent and fuel; methanol is used as a solvent, fuel, and reagent in industrial chemical processes.
- *Aldehydes* can be found in resins, disinfectants, biocides and furniture. Formaldehyde is used as a disinfectant, bactericide, preservative, reagent, and glue in both wall and ceiling panels and wood-based panels; acetaldehyde, as well as being used as a reagent in industrial synthesis processes.

VOCs are widely used in the wood sector for painting and other finishing processes, as solvents in paint formulations to improve the application characteristics, such as flow and levelling, and to enhance the drying time.

The negative impacts of VOCs include ground-level ozone formation, which is a key component of smog and contributes to respiratory problems in humans. VOCs can also have toxic effects on the central nervous system, causing headaches, dizziness, and nausea.(Y. Yang et al., 2019; Z. Zhang et al., 2018) Long-term exposure to high levels of VOCs has been linked to cancer and other serious health problems (Li et al., 2023).

GREENHOUSE GASSES (GHG)

A greenhouse gas (GHG or GhG) is a gas that absorbs and emits radiant energy within the thermal infrared range, causing the greenhouse effect.

Greenhouse gases are compounds that can trap the atmospheric heat and contribute to the greenhouse effect. The primary greenhouse gases in Earth's atmosphere are water vapor (H_2O), carbon dioxide (CO_2), methane (CH_4), nitrous oxide (N_2O), ozone (O_3), and fluorinated gases. CO_2 is the most abundant and well-known greenhouse gas, and its primary source is the burning of fossil fuels for energy.

Methane is released during the production and transportation of coal, natural gas, and oil. Nitrous oxide is produced from agricultural and industrial activities, as well as from burning fossil fuels. Fluorinated gases are synthetic gases that are used in a variety of industrial processes and are potent greenhouse gases but are much less abundant than the other three. The build-up of these gases in the atmosphere leads to an increase in the average global temperature, which can result in long-term changes to the planet's climate and ecosystems (Shukla P.R. et al., 2019).

The effects of greenhouse gases on human health can be significant and far-reaching. Rising global temperatures can lead to more frequent and intense heat waves, which can increase the risk of heat-related illnesses and death, particularly for vulnerable populations such as the elderly and people with pre-existing medical conditions (Kuklinska et al., 2015). Climate change can also exacerbate air pollution, which is a major contributor to respiratory and cardiovascular diseases. In addition, the spread of disease-carrying insects, such as mosquitoes, to new areas can increase the incidence of infectious diseases such as malaria and dengue fever. Rising sea levels can also result in flooding and contamination of drinking water supplies, putting people at risk of waterborne illnesses (Gulia et al., 2022). Also, changes in the timing and availability of food and water can disrupt the food security and health of communities, particularly in developing countries.

Overall, the impacts of greenhouse gases on human health can be significant and highlight the importance of reducing emissions and taking action to mitigate the effects of climate change.

PARTICULATE MATTER (PM)

Particulate matter is a mixture of solid particles and liquid droplets that are frequently found in the air, and they can give a significant impact on the environment and human health. PM2.5 and PM10 refer to the size of the particles, with PM2.5 being finer and potentially more dangerous. Fine particles (PM2.5) can penetrate deep into the respiratory system and cause or worsen respiratory and cardiovascular diseases, such as asthma, bronchitis, heart attacks, and stroke. Long-term exposure to PM2.5 has also been linked to decreased life expectancy (Hu et al., 2023).

In addition to its impacts on human health, particulate matter can also harm the environment. Fine particles can reduce visibility and affect natural habitats and wildlife, while larger particles can damage crops and interfere with rainfall patterns. PM also contributes to the formation of acid rain, which can harm soil and water quality. Acid rain, in fact is a type of rain that has a pH lower than 5.6, caused by the emission of sulphur dioxide and nitrogen oxides into the atmosphere, which react with the atmosphere to form sulfuric and nitric acids. PM can be one of the components of acid rain, but it also includes other sources such as dust, pollen, and sea spray. The effects of acid rain and PM can include damage to crops, trees, buildings, and other structures, as well as respiratory and other health problems for humans and wildlife.

The primary sources of particulate matter include power plants, transportation (cars, trucks, and buses), industry, and agricultural and natural dust. To reduce the impacts of PM, it is important to limit emissions from these sources and to promote the use of cleaner technologies and fuels.

2. BACKGROUND ON VOCs MANAGEMENT

From the beginning of scientific research into the management and mitigation of environmental risks and impacts, the best technologies for VOC abatement have been investigated. Studies show that industrial processes account for 16% of total global VOC emission, biofuels (18%), biomass combustion (14%) but the major contribution comes from combustion of fossil fuels (49%) (Gupta & Modi, 2018). Especially for the industrial application, different technologies are available (Fig.1). Many of those, currently in use, are the result of time-tested abatement systems, such as regenerative thermal oxidizers (RTO).

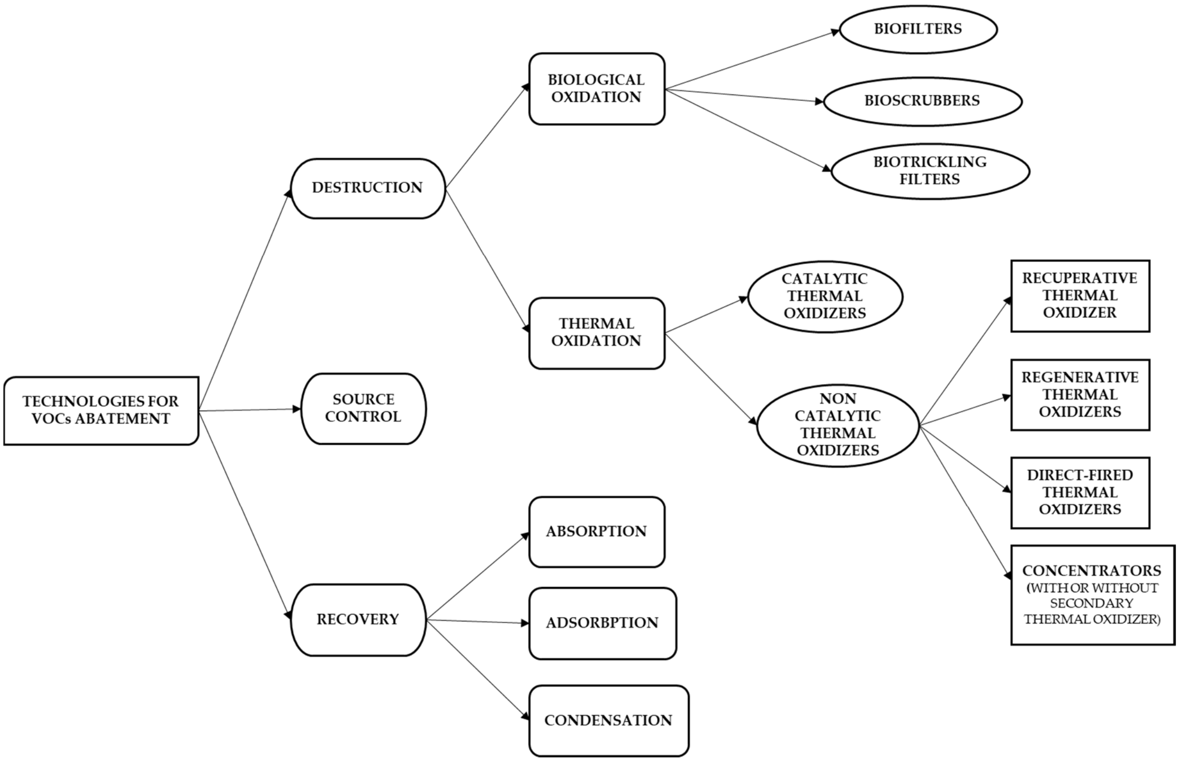


Fig. 1 *VOCs abatement technologies for industries*

The regenerative and recuperative energy recovery plants are the most currently used in the industries because they allow to reduce the energy demand instead of the traditional thermal oxidizers, (Amelio & Morrone, 2007; Salvador et al., 2005). Therefore, they are used by companies that have been active for a long time.

Nowadays the modern industrial plants and producers of industrial VOC emissions are increasingly searching for methods to treat emissions at an acceptable level and with reduced operating expenses (OPEX) (Brummer et al., 2022). Although research is now specializing in the design of better abatement systems, such as catalytic, adsorption, concentrator ones (Kamal et al., 2016; Qiang et al., 2020; Sultana et al., 2015; Tomatis et al., 2016; C. Yang et al., 2019; W. Zhang et al., 2022; Zhu et al., 2020), abatement systems with high maintenance and operating costs despite high efficiencies are still in operation. From this point of view, sustainability research is also involving Life Cycle Assessment (LCA), such as by (Tomatis et al., 2019) where a LCA of three thermal oxidizers for VOCs oxidation is conducted. It has also been emphasized that the electricity and fossil fuel are the main contributors to the impact of all oxidizers.

In this context, the present research work is based on an innovative approach that aims to consider biomass as a thermal source for VOC abatement, instead of the fossil fuels.

3. INDUSTRIAL PROCESSES THAT USING VOCs: AIR QUALITY REGULATIONS

To reduce the negative effects of VOCs, it is important to limit exposure by using products that have low levels of VOCs and properly ventilating areas where these products are used. Additionally, regulation of VOC emissions from industrial sources is important for protecting both the environment and public health.

3.1. TYPE OF EMISSIONS

DUCTED EMISSIONS

Ducted emissions refer to the release of pollutants into the atmosphere through a duct or pipe. These pollutants can come from various sources such as industrial processes, power plants, and transportation vehicles.

FUGITIVE EMISSIONS

Dust produced by sources that introduce solid particles into the atmosphere is defined as diffuse or fugitive emissions. Several sources contribute significantly to atmospheric emissions of solid particles. Major sources of diffuse dust include wind erosion of exposed surfaces, paved and unpaved roads, construction work and other industrial activities, especially quarries and mines. According to a study conducted by the United States Environmental Protection Agency (U.S. EPA, 1998), emissions from diffuse sources account for 89% and 66% of all PM10 and PM2.5 emitted into the atmosphere.

Exposure to airborne dust, whether occupational or non-occupational, poses a health risk to those exposed. Currently, epidemiological studies have shown a causal relationship between exposure to high levels of dust and the development of respiratory disease, heart disease, stroke, changes in the immune system, and lung cancer (Chen & Hoek, 2020; Yuan et al., 2019).

The diffusion of particulate matter in the atmosphere is also associated with several important environmental concerns, leading to adverse effects on ecosystems, climate and microclimate, visibility and air permeability, and material degradation. From an environmental perspective, particulate matter is one of the six most widely distributed substances in the atmosphere. Occupational exposure to particulate matter is currently regulated by which imposes an obligation on employers to assess worker's exposure and to take all necessary risk mitigation measures. In fact, this decree establishes concentration limits for a limited number of chemical substances in accordance with standards issued on a European scale.

Italy's recently implemented European Air Quality Directive through Legislative Decree 155/2010 sets concentration limits for PM10 and PM2.5. Compliance with these limits is verified by a complex network of instruments spread across the country and administered by each region. Data collected by instruments, often combined with simulation results using appropriate mathematical models, allows monitoring of air quality conditions.

In addition to indoor PM contamination, it is important to consider VOC contamination. In fact, several studies (Adamová et al., 2020; Guo et al., 2004; US Environmental Protection Agency, 2022) have shown that VOCs indoors can be present in quantities as much as 10 or 20 times higher than those found outdoors, in the presence of indoor emissive sources and reduced air recirculation.

VOCs can cause two types of toxicity:

- acute (short-term) toxicity, that is the result of a single exposure or several repeated exposures occurring throughout the day. Effects include headaches, nausea, eye, throat and nose irritation, dizziness, and asthma.
- chronic (long-term) toxicity, which is the result of long-term exposure. Effects include damage to the central nervous system, kidneys, or liver.

Furthermore, some VOCs have even been classified by the IARC (International Agency for Research on Cancer) as carcinogenic: these include formaldehyde and benzene (IARC, 2022).

3.2. KEY ENVIRONMENTAL REGULATIONS

EUROPEAN

- (Directive EU n. 2284, 2016) - On the reduction of national emissions of certain atmospheric pollutants, amending Directive 2003/35/EC and repealing Directive 2001/81/EC.
- (Directive EU n. 75, 2010) - On industrial emissions (integrated pollution prevention and control) and BAT (Best Available Technologies).
- (Directive EU n. 2193, 2015) - On the limitation of emissions of certain pollutants into the air from medium combustion plants.
- (Directive EU n. 2284, 2016) - On the reduction of national emissions of certain atmospheric pollutants, amending Directive 2003/35/EC and repealing Directive 2001/81/EC.
- European Pollutant Release and Transfer Register (E-PRTR) (Regulation EU n. 166, 2006) (European Environment Agency, 2022) – is a database that provides information on releases of pollutants into the environment and transfers of waste from industrial facilities. Under the E-PRTR Regulation, facilities in EU Member States are required to annually report on their releases and transfers of specified pollutants. The information is made publicly available on the E-PRTR website to promote transparency and accountability.
- (Directive EU n. 98, 2008) - End-of-waste criteria - Specify when certain waste ceases to be waste and becomes a product, or a secondary raw material.

ITALIAN

- (D.Lgs. n. 152, 2006) Environment Act - Transposes European legislation and integrates with the Italian one in a consolidated text. It sets regulations on soil and water protection, waste management, air pollution reduction, environmental impact assessment and compensation for environmental damage. The decree has been modified several times over the years, the latest being introduced by Legislative Decree No 21 of 2018. Part Five of the TU concerns 'regulations on air protection and reduction of emissions into the atmosphere'. In detail, Title I regulates 'prevention and limitation of atmospheric emissions from plants and activities' by establishing 'emission values, prescriptions, methods of sampling and analysis of emissions, and criteria for assessing the conformity of measured values'. Art. 275 deals specifically with VOC emissions.
- (D.Lgs. n. 46, 2014) A.I.A. Integrated Environmental Authorization - is the permission that some companies need to achieve to meet the principles of integrated pollution prevention and control (IPPC-IED) dictated by the European Union.
- (D.Lgs. n. 81, 2008) Safety and security in workplaces Act – regulates the protection of workers' health and safety in the workplace.
- (D.Lgs n. 264/2016, 2016) 'Regulation containing indicative criteria to facilitate the demonstration of the existence of the requirements for the qualification of production residues as by-products and not as waste'.
- UNI EN ISO 17225 series. Provides the general requirements and specifications for solid fuels and defines the classifications of wood pellets, wood briquettes (or logs), wood chips, firewood, non-wood pellets and, finally, the classes of non-wood briquettes. Specifically, 17225-4 establishes the specifications and classification of wood chips.

4. INDUSTRIAL ABATEMENT TECHNOLOGIES AND RAW WASTE MATERIALS MANAGEMENT

As already mentioned, VOC abatement refers to the process of reducing or removing the emissions of VOCs into the air. Abatement measures can include source control, such as using low-VOC products, and air treatment technologies, such as carbon adsorption or oxidation. The goal of VOC abatement is to reduce the levels of these compounds in the atmosphere, and to improve air quality.

The following paragraphs describe the most common biomass and abatement system.

4.1. REGENERATIVE THERMAL OXIDIZERS (RTO)

A Regenerative Thermal Oxidizer (RTO) is a device specifically designed for air pollution control and is used for the abatement of volatile organic compounds (VOCs) and hazardous air pollutants (HAPs) from industrial processes. It works by heating the contaminated air stream to high temperatures (typically between 800-1200°C) in order to cause the oxidation of the VOCs and HAPs. The heat energy generated during the oxidation process is recovered and reused to preheat the incoming contaminated air stream, making the RTO a highly energy-efficient solution for VOC abatement. The outlet purified air carbon dioxide (CO_2) and water vapor (H_2O) is composed mainly of released into the atmosphere.

The RTO is a well-established system that is on the list of Best Available Technologies (BAT) available to be used for pollutant abatement according to European legislation. This list is periodically revised, and this equipment remains one of the most widely used, especially for its high destruction efficiency 95-99%.

In addition, if well managed, it allows a considerable reduction in the consumption of the non-renewable energy vector (methane) used to fuel the flame. In fact, if the VOC concentration is greater than 1.5 g/Nm^3 the system enters self-sustaining mode, and the combustion chamber is maintained at the optimal temperature thanks to the thermal energy provided by the spontaneous combustion of the VOC.

Pollutant Destruction Phase

- Firstly, a high-pressure supply fan forces exhaust fumes to the RTO.
- Inlet switch valves direct the pollutant-laden air into one of the energy recovery canisters.
- The air continues to travel from the valve assembly up through the first heat exchanger canister where heat is absorbed from the ceramic media.
- The preheated air moves into the combustion chamber and is held at an elevated temperature close to that required for oxidation.
- The pollutant is destroyed while in the combustion chamber.

Clean Air Cycle

- After leaving the combustion chamber, the hot, cleaned air flows through a second energy recovery sector, where ceramic media absorbs the heat generated during thermal oxidation.
- Finally, the clean, cooled air is directed into the atmosphere via the outlet switch and finally the chimney.

4.2. VOC'S CONCENTRATORS

These devices called "rotary concentrator" are used mainly to treat air streams that include VOCs. The solvents are first held in an adsorbent structure before being released at a considerably lower flow rate than they were at first, usually for burning as the next step in the treatment process (in rare cases, it may be convenient to condense and recover the solvent). As a result, there is a significant economic benefit, which essentially entails a smaller combustion plant and lower operational expenses. In actuality, the combustor operates at a very high concentration with a very tiny flow. Thus, it is usually easy to keep the fuel level at a point where the proper process temperatures can be maintained without the need for more fuel.

The concentrators typically use adsorption, absorption or thermal desorption techniques to trap and concentrate VOCs from a polluted airstream. They are used in a variety of applications, including environmental monitoring, indoor air quality assessment, and industrial process control. The efficiency and selectivity of VOC concentrators can vary depending on the specific design and the target compounds. Combining a VOC concentrator with a thermal oxidizer can effectively treat and eliminate high concentrations of volatile organic compounds. In fact, the concentrator collects and concentrates the target compounds, which are then fed into the thermal oxidizer. This combination is commonly used in industrial settings where large amounts of VOCs are generated and must be eliminated in order to meet environmental regulations and minimize air pollution.

The transfer of the organic substances from the main flow to the reduced flow takes place through a temperature-regulated adsorption process by the zeolites. The effluent stream to be treated, after a filtration process to remove coarse dust, is passed through a sector of the concentrator drum in slow, continuous rotation. The purified air after passage is sent directly to the stack. For effective adsorption, the flow must be at a low temperature, equal to ambient temperature or slightly higher, at most around 40°C (if the effluent is too hot, it must be cooled appropriately by a heat exchanger). Desorption occurs instead by passing the rotor section into a subsequent flow at a higher temperature, between 180° and 220°C, usually achieved by an auxiliary burner (i.e. RTO). The boiling point of the VOCs must be below this temperature, otherwise de-sorption cannot take place. For proper operation of the concentrator, there must be no or only trace amounts of high-boiling VOCs in the emissions. The concentration of VOCs in the inlet can be between values very close to 0 and an upper limit around 1.5 g/Nm^3. The lower the inlet concentration, the higher the achievable concentration ratio, from about 15:1 to 5:1. The outflow from the desorption, hot and concentrated, is sent to the regenerative combustor, passing through the heat recovery chambers which heat it up again (giving up the heat accumulated through the passage of exhaust gases in a previous phase of the cycle). In the combustion chamber, VOC oxidation takes place at a temperature of around 850° - 1000°C. The flue gases are then passed into one of the recovery chambers and sent to the stack. Thanks to the suitably reduced and concentrated flow, the combustor can be much smaller than would be necessary without a concentrator, while, once the operating temperatures are reached with the aid of auxiliary burners, the oxidation process can take place in self-sustaining mode, without additional fuel input.

NON-RENEWABLE SOURCES CONSUMPTION

The use of methane in thermal oxidizers can have several benefits, including energy efficiency and cost savings compared to other fuel sources, as well as reduced emissions of harmful pollutants (Tomatis et al., 2019). However, also requires careful consideration of safety and environmental regulations, as well as the potential release of other pollutants such as nitrogen oxides (NOx) during the combustion process. Furthermore, in the case of RTOs, if the system does not get into the self-sustaining mode, the methane must provide for the maintenance of the optimal temperature and this causes its high demand (Cannon, 2003).

4.3. BIOMASS BOILERS

When biomass is burned or consumed, the carbon combines with oxygen in the air to generate carbon dioxide, which is released into the atmosphere after being transformed into other fuel types (i.e. charcoal, ethanol, and methane). The amount of carbon dioxide produced, if entirely burned, is equal to the amount drawn from the atmosphere during the growing stage (Saidur et al., 2011). Therefore, biomass can be thought of as a carbon sink and there is no net input of CO_2.

Biomass thermal treatment refers to the process of heating organic materials such as virgin wood, or other plant-based material, to produce heat, electricity, or biofuels. This process typically involves the combustion of this biomass to generate steam, which is then used to power a turbine or generate electricity. The heat generated can also be used for space heating or process heat in various industries. The biomass thermal treatment is considered a renewable energy source, as it utilizes waste material to produce energy and reduces greenhouse gas emissions compared to fossil fuels.

5. CASE STUDY

The co-financing partner of the PhD project (Pan Eco S.r.l.) deals with environmental and occupational safety consultancy and is active mainly in the province of Ancona, with a heterogeneous client base.

This background highlighted a common problem, especially in small and medium-sized companies: the high consumption of a non-renewable resource (i.e., methane) for supplying thermal oxidisers, where self-sustainability is not possible.

This issue motivated this PhD research, to try to find a possible solution. Even though the thermal oxidation technology is well established and has excellent abatement efficiencies, methane consumption often becomes too high, which also causes a considerable increase in operating costs.

The selection of the company, to be used as a reference point, was based on the following steps.

Firstly, were identified the sectors most affected by using solvents, such as newspaper printing, woodworking, and plastics production.

Secondly, were investigated the types and amounts of waste products to be valorised for energy recovery.

The aim was to find the right balance between the amount of solvents used and the amount of raw material waste produced. This second point was considered to encourage the reuse of waste in a perspective of circular economy and sustainability.

5.1. KEY COMPANY INFORMATION

Industrial sector: wooden furniture and fixtures production.

Address: Castelfidardo (AN).

Number of employees: 220.

Reference regulations for emissions: Environmental Integrated Permit (A.I.A).

Total area: 56000 m^2.

Average annual number of parts produced: 65000.

Maximum theoretical solvent input: 650 ton/year.

5.2. MANIFACTURING PROCESSES

The complete manufacturing process of a wooden furniture element or component is very articulated. In the initial phase, the virgin boards or panels are taken from the warehouse to the machining departments, where they are sized according to their use. Thereafter, the parts are shaped more accurately using pantographs, edging machines, cutting-off machines, plane moulders and frame edgers. Afterwards the parts are taken to the painting departments, in this company there are two work areas where these operations take place.

Currently, there are three different types of coating that can be used to cover the raw piece of wood:

- *solvent-based coatings*, which consist of polymer-based products such as polyester, polyurethane, vinyl acetate.
- *water-based coatings*, which contain a high percentage of water (up to 80 per cent) replacing the solvent.
- *powder coatings*, in which powder is sprayed onto the workpiece using an ionized air current, which is attracted to the part that has been charged by the opposite sign.

Solvent-based coatings are used in this case as they provide a better hold.

In the painting departments are located: closed automated painting stations, open manual painting cabins and painting carousels, as can be seen in below images (Fig. 2, 3, 4,5).

Fig. 2 *Carousel 1/2*

Fig. 3 *Carousel 2/2*

Carousels are painting systems in which workpieces are placed or are held in suspension to be sprayed by the machines. Unfortunately, this operation is more wasteful regarding the raw materials and VOCs emitted than spray booths.

Fig. 4 *Manual painting cabin*

In the spray booths, the coating is applied with manual spraying systems. During the coating process, air polluted by paint particles and/or evaporated solvents is extracted through a grid set in a tank located beneath, which contains water, or in a vertical wall where a veil of water passes through. The air then flows into the tank and the heavier solid particles are deposited.

Fig. 5 *Automatized coating station.*

In automated painting stations, the parts are placed on a conveyor belt and sent to the closed booth where the spray coating takes place. In the booth, the polluted air is extracted directly without any excessive dilution with ambient air.

As well as this company, many others in the same sector also use these old open equipment and installations, mainly because they perform their function very well. Unfortunately, non-compartmentalised workstations cause the dispersion of pollutants into the environment and inhalation risks for the employers. In addition, the polluted air extracted is diluted by clean atmospheric air. This causes a high increase of costs for the realization and maintenance of abatement plants.

5.3. OVERVIEW OF THE VOCs ABATEMENT SYSTEM USED AND RAW WASTE MATERIAL PRODUCED

The VOCs abatement system used in the factory is a regenerative thermal oxidizer (RTO) with two towers. As mentioned previously, this type of equipment is specifically made for industrial sectors that use a large amount of solvents or emit a lot of chemical compounds in the atmosphere. Figure 6 shows the RTO that is installed in the factory with his pre-scrubber. In fact, the latter is used to clean the airflow from the dust.

Fig. 6 *Regenerative Thermal Oxidizer and wet scrubber*

The Integrated Environment Authorization (A.I.A.) permits the company for a specific amount of polluted air that can be treated by RTO, depending on the VOCs produced and the capacity of the plants using them (carousels, painting stations etc.). The following table provides the A.I.A. permitted parameters and limits concerning emission of pollutant in the atmosphere.

Abatement System	RTO - Regenerative Thermal Oxidizer			
Flow [Nm^3/h]	40000			
Section Area [m^2]	0.8			
Height above ground [m]	10			
Temperature [°C]	70			
Monitoring parameters	Total Particulates	VOC (as TOC)	Nitrogen Oxides - NO_2	Carbon Monoxide CO
Limit values [mg/Nm^3]	6	75	100	100
Mass Flow [g/h]	240	3000	4000	4000

Tab. 1 *A.I.A. permitted parameters and limits of the case study company.*

The RTO plant consists of two towers connected at the top by a combustion chamber, each of which contains ceramic material that cyclically accumulates and releases heat. A fan that is built to handle the system's pressure drops extracts the dirty air. When there is a changing flow rate, an exhaust adjustment system (inverter) is added to optimize energy use. The cold air is passed through the first tower, which includes ceramic material, to be treated from the bottom up. It uses the treated outgoing effluent to absorb the heat that the ceramic accumulated during the previous cycle. Purified hot air from the combustion chamber, where it collects heat, travels through the second tower. The first tower is purged and cleaned from pollutant residues to prepare it for the effluent outflow in the next cycle. The purging is useful as the chamber previously contained the incoming polluted effluent. A series of valves, specially designed and tested for safety and security, switches the inlet and outlet of the effluent into the reactors, thus realising a cyclic process. This thermal exchange system, obtained by using ceramic masses, allows potentially high heat recovery.

This abatement system was installed in the company according to the bets available technologies. Unfortunately, the VOC concentration in the inlet flow very often is not high enough to ensure self-sustaining combustion. Consequently, the optimal combustion temperature in the chamber is not maintained (above 750- 900°C). This is why methane consumption is very high, because it keeps the burner flame at the correct operating rate. In the preliminary stages of the company's analysis, methane consumption was also investigated. The volume observed during the monitoring years is 53000-55000 Sm^3 per year in average, only for the RTO power supply.

The opportunity to introduce concentrators has been evaluated but, unfortunately, in this particular case it is not possible to concentrate all VOCs species because there could be issues with the regeneration of zeolite and correct implementations of the layout. Therefore, VOC concentrators cannot be installed before the RTO.

Furthermore, the pre-scrubber is used to preserve the thermal oxidizer both from a mechanical and process point of view, reducing the concentration of types of pollutants such as organic silicone compounds, inorganic acids, inorganic bases, aerosol, dust, painting overspray, oily mist and/or condensate droplets.

As regards the production of virgin wood waste material, as can be expected, there are large quantities produced. Especially from the initial stages of cutting, shaping and sanding. This type of material is not considered a waste, strictly defined, but a by-product. The definition of by-product has been found in Italian legislation since the emanation of D.lgs. 152/06 and in EU legislation since the publication of Directive 98/2008/EC on waste. Italy has introduced this definition in advance of the EU regulations. A by-product is a residue of a production cycle that is not classified as waste and is not subject to all the regulatory obligations associated with waste management but can be used and traded as an asset (FederlegnoArredo, 2017).

6. PROPOSED SYSTEM

As mentioned earlier, the core of the PhD was to research an alternative equipment for VOCs abatement and thermal recovery of raw material waste. The system uses the raw waste biomass combustion as a heat source for the thermal destruction of VOCs in the air flow extracted from the workstations. In this way, the methane consumption, as an energy vector, is almost eliminated because it is only used to power the flame to burn the biomass.

The flowsheet of the proposed system is shown below (Fig. 7).

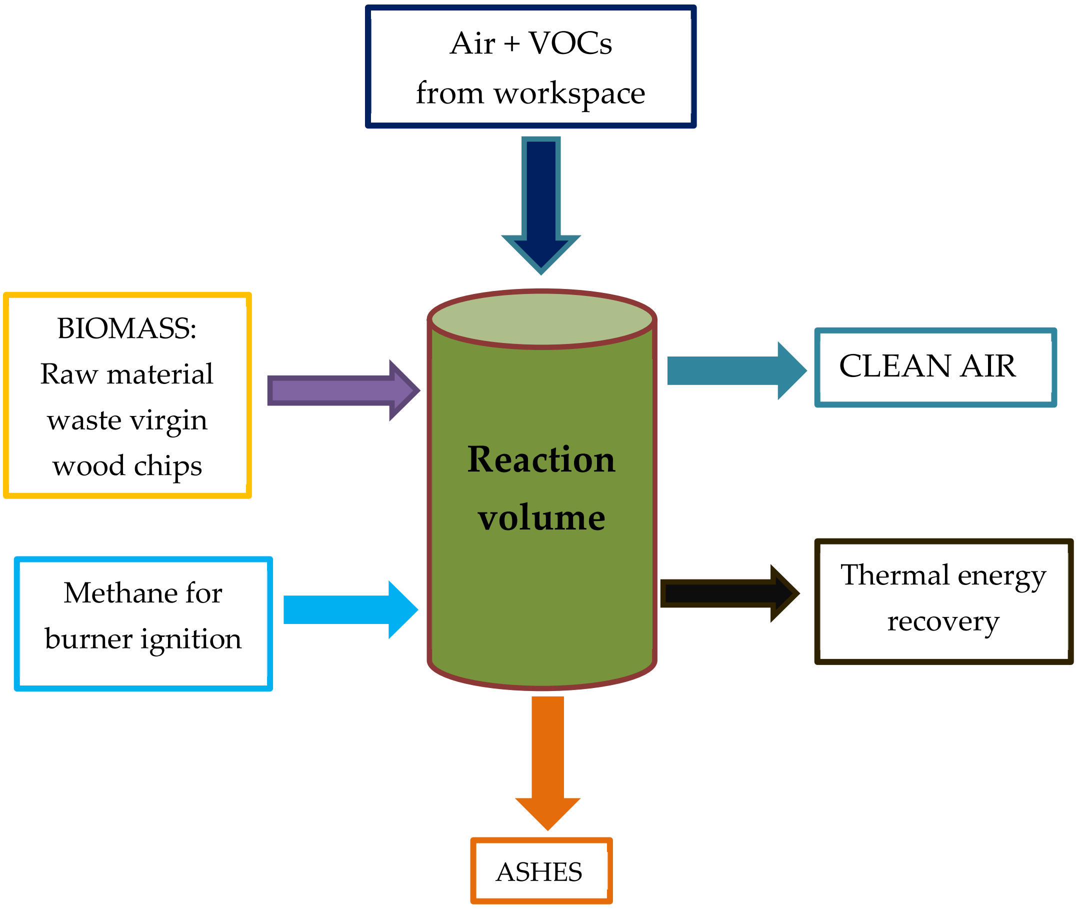


Fig. 7 *Flowsheet of the proposed system*

7. EXPERIMENTAL PROTOCOL

The experimental phase consisted of a series of sampling campaigns at specific VOCs detection points to obtain the mass balance of pollutants from the solvent use areas to the thermal treatment system outlet. The sampling and related analyses served as preliminary data to characterise most of the VOCs involved in the processes and to determine the input parameters to be used as feeds for the proposed innovative system.

7.1. SAMPLING CAMPAINGS

The measurement campaigns were carried out for two years (2020-2021). Two sets of samplings were made during the spring-summer and autumn-winter periods to account for the fluctuation of the production and variation of the environmental conditions. For the year 2020, only two measurement campaigns could be carried out due to the CoVid-19 pandemic restrictions.

Due to the impossibility of analysing the whole emission from the stack in each period, to define the characteristics of a ducted emission, a small part of it, called a sample, is examined.

For the small sample of fluid taken to be representative of the entire quantity emitted from the stack, that fluid must present:

- physical characteristics and homogeneous composition throughout the section of duct in which the sampling outlet is positioned;
- steady-state flow (physical characteristics and composition constant over time).

If this is not the case, the fluid sample taken will have different characteristics to those (average) of the entire quantity of fluid emitted from the stack; therefore, the determinations made on the sample will consequently provide different and incorrect information with respect to the entire quantity of fluid emitted from the stack.

The current UNI EN ISO 16911:2013 standard, indicates that to carry out sampling with acceptable accuracy it is essential that the flow of gas within the duct is sufficiently stationary and homogeneous; for this to be possible it is necessary that the section of duct being measured meets certain requirements. Sampling points must be in straight sections of pipeline with a regular cross-section (circular or rectangular), preferably vertical, away from obstacles, curves or any discontinuity that may influence the movement of the effluent. To guarantee the condition of stationary condition the location of the sampling point must respect the conditions imposed by the reference technical standards (UNI 10169:2001, UNI EN 15259:2008) i.e., at least 5 hydraulic diameters downstream and at least 2 hydraulic diameters upstream of any discontinuity.

The hydraulic diameter (Dh) is a measure of the size of a pipe or channel used to transport fluid. It is defined as four times the flow area of the pipe divided by its wetted perimeter.

$$Dh = \frac{4A}{p}$$

Where:

A = cross-sectional area
p = wetted perimeter of cross-section

In case of circular ducts, the Dh is the same as the geometric internal diameter of the section.

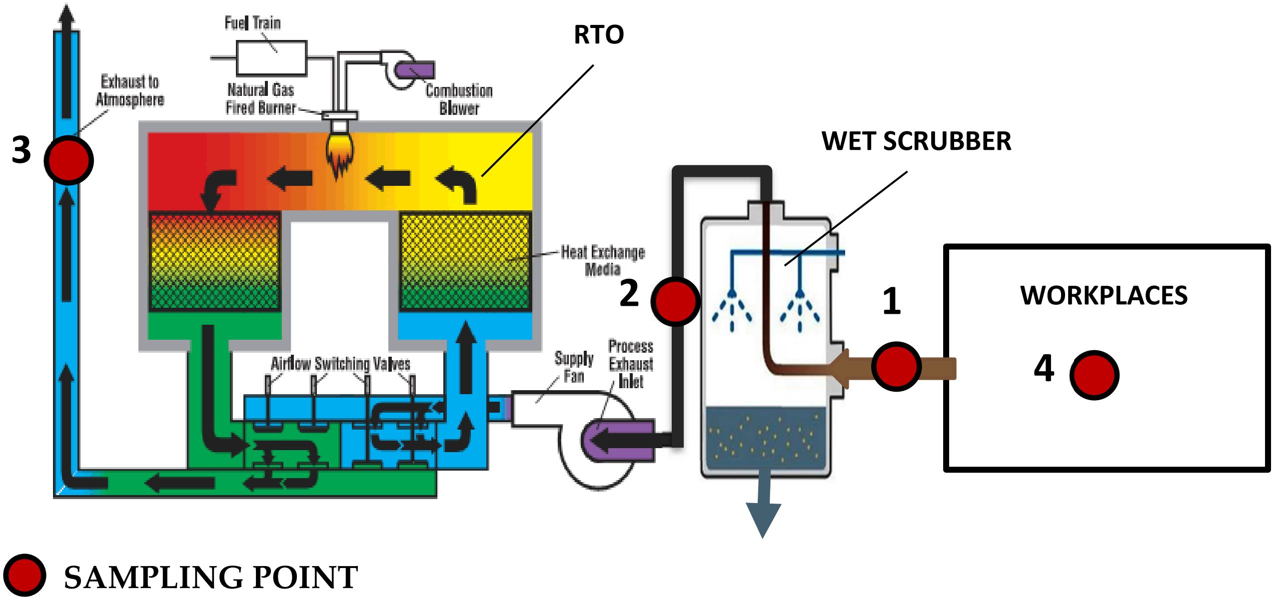


Fig. 8 *Flow-chart of the VOCs emission (some images are taken from Google Images)*

Point n. **1 -** Outlet flow from workplaces (Fig. 9)

Point n. **2** - Outlet flow from wet pre-scrubber (Fig. 10)

Point n. **3** - Outlet flow from RTO (Fig. 11)

Point n. **4** - Workplaces environment (Fig. 12)

7.1.1. OUTDOOR SAMPLING

Outdoor sampling was used to obtain the mass balance, in terms of solvents, of the abatement system. As already mentioned, the company is obliged by regulation to monitor the pollutants leaving the stack every year. But no upstream values are required by law, except for the annual E-PRTR declaration on solvent consumption. This reporting, however, concerns quantities that result from inaccurate approximations from the safety data sheets of the products used. Therefore, in order to get an accurate estimation of the amount of solvents involved, the delivery pipes were sampled.

Fig. 9-10 *Sampling points 1 and 2*

Fig. 11 *Sampling point 3*

The following equipment was used for sampling:

- SKC AirCheck 3000 sample pump (1lt/min);

- Charcoal Sorbent Tubes SKC 226-09;

- Polaris FID TOC analyser T0574-PF-300;

- Horiba PG-250 Portable Gas Analyzer

Air sampling was done with pumps set at a flow rate of 1 lt/min and pollutants were sampled and enriched using activated carbon adsorbent vials. The sampling time was 30 minutes for each point. After each sampling, the vials were placed in a refrigerated container for transport to the laboratory.

At the same time, the Polaris FID analyser was used to determine total organic carbon (TOC) and the Horiba analyser was used to determine Nitrogen Oxide (NOx), Sulphur Dioxide (SO_2), Carbon Dioxide (CO_2), Carbon Monoxide (CO), and Oxygen (O_2).

7.1.2. INDOOR SAMPLING

Workplace air sampling was done according to the UNI EN 689 Standard for the assessment of occupational exposure to chemical. These can be performed using Radiello passive sampler positioned in the centre of the environment on a stand at a height of 1.5 m from the ground and well away from sources of turbulence (Fig.). The duration samplings were 8 hours, because this time is representative of the work shift and, therefore, of the potential weighted average exposure over eight hours (TWA) required for a reasonable comparison with Threshold Limit Values – Time Weighted Average (TLV-TWA).

Fig. 12 *Sampling point 4*

Radiello (Fig. 13) is a passive sampling unit for air quality monitoring that requires several components to function. The basic components are the support plate, the diffusive body, the adsorbent element, and the barcode label to make the sample traceable.

Fig. 13 *Radiello components*

7.2. LABORATORY CHARACTERIZATION

The analytical methods are specified in the 'SNPA Guidelines No. 16/2018' (Clerici L. et al., 2018). In this document there is a guidance on the types of media to be used for sampling and guidance on laboratory protocols for analysis.

As already mentioned, once the sampling is complete, the vials are closed at the ends and placed in a refrigerated container. The samples /Fig. 14) are transported to the laboratory as quickly as possible, and the analytical steps immediately begin.

The analytical methodology for desorbing volatile organic compounds (VOCs) from coal vials typically involves the following steps:

1. *Sample preparation:* This step is crucial for obtaining a representative sample for analysis. The coal in the sorbent tubes (Fig. 15) should be crushed and homogenized to a fine powder to ensure a uniform sample. Depending on the size of the vials, this can be done using a mortar and pestle, a ball mill, or a laboratory grinder.

Fig. 14 *SKC 226-09 Charcoal Sorbent Tubes*

After that, the coal must be transferred in Vial container as shown in Fig. 15.

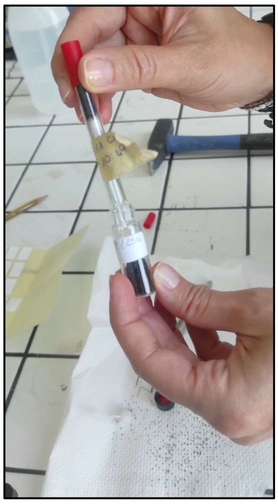


Fig. 15 *The coal is transferred in a Vial container.*

2. *Desorption, purification, and concentration:* There are two main methods for desorbing VOCs from coal: solvent extraction and thermal desorption.

   In this case was used the **solvent extraction**. An appropriate solvent is used to dissolve the VOCs from the coal matrix, which are then transferred to a new container for further analysis. Common solvents used for VOCs extraction include dichloromethane, carbon disulphide, ethyl acetate, and hexane. In this case was used the **Carbon disulphide** (CS_2). 2 ml of this compound is added to coal dust (Fig. 16-17), and the vial is stirred with ultrasound equipment for 5 minutes.

   After the VOCs are desorbed, they are purified and concentrated using a Liquid-liquid extraction (LLE). An extraction solution is prepared consisting of CS_2 and Chlorobenzene (C_6H_5Cl), which is the internal standard. The quantities are 10 µl of C_6H_5Cl in a 4 ml concentration of CS_2. This solution is necessary both for the desorption of VOCs and for the correct visualization of the peaks in the chromatogram. The samples are stirred again for 30 minutes.

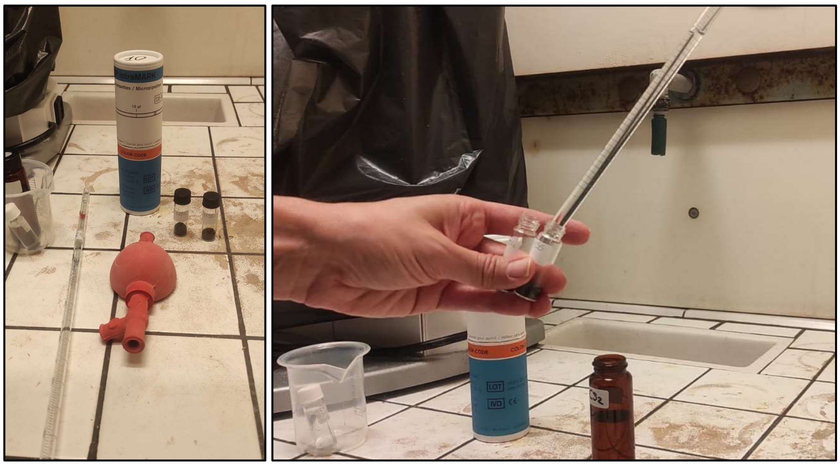


Fig. 16-17 *Addition of extraction solution.*

3. *Analysis:* The purified and concentrated VOCs are analyzed using gas chromatography with flame ionization detection (GC-FID) to identify and quantify the individual compounds. A 1 µl of the sample solution is then collected and injected into the GC (Fig. 18).

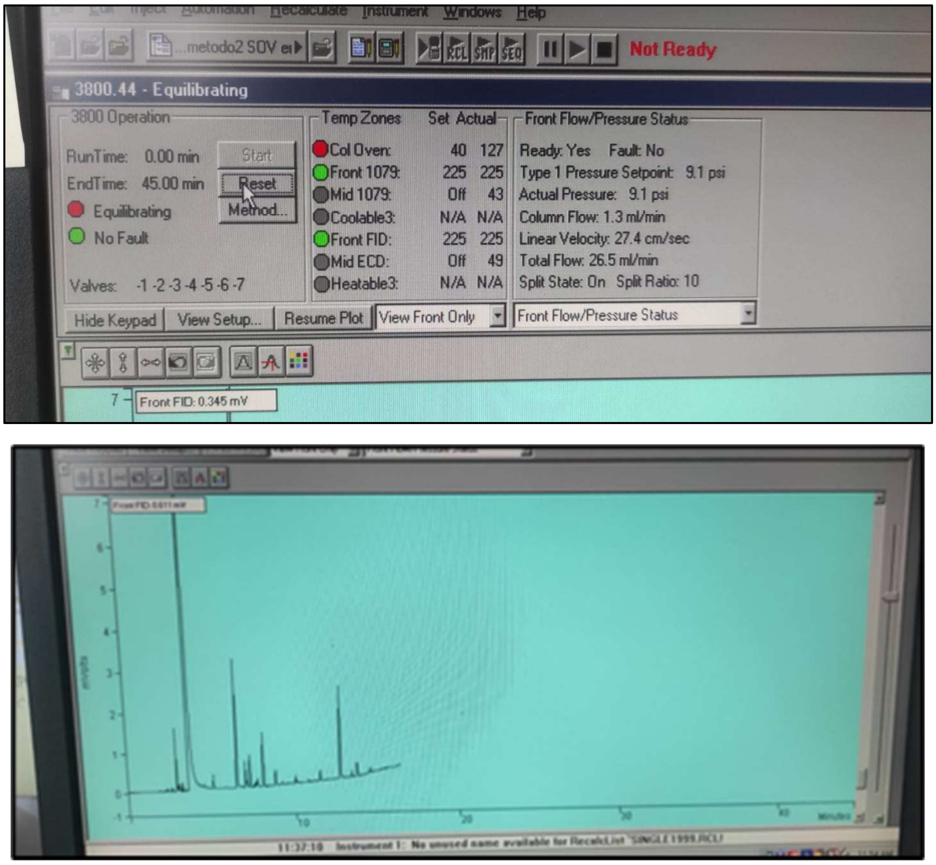
Fig. 18 *GC-FID CP-3800.*

The gas chromatographic analysis was carried out under operating conditions:

- SPB-1 bulk silica column 30 metres in length x 0.32 mm in diameter
- Splitter injector 1:20 (225°C)
- FID detector 225°C
- Carrier gas He 70 KPa
- Thermal programme from 40°C for 3' up to 180°C for 10' (with gradient of 5°C per minute)

Relative concentrations were measured using the external standard method.

4. *Data interpretation:* The analytical data is interpreted to determine the presence, concentration, and identity of the VOCs in the coal sample (Fig. 19-20)



3800.44 - Equilibrating

3800 Operation

RunTime: 0.00 min
EndTime: 45.00 min
Equilibrating
No Fault
Valves: -1 -2 -3 -4 -5 -6 -7

Temp Zones	Set	Actual
Col Oven:	40	127
Front 1079:	225	225
Mid 1079:	Off	43
Coolable3:	N/A	N/A
Front FID:	225	225
Mid ECD:	Off	49
Heatable3:	N/A	N/A

Front Flow/Pressure Status

Ready: Yes Fault: No
Type 1 Pressure Setpoint: 9.1 psi
Actual Pressure: 9.1 psi
Column Flow: 1.3 ml/min
Linear Velocity: 27.4 cm/sec
Total Flow: 26.5 ml/min
Split State: On Split Ratio: 10

Front FID: 0.345 mV

Fig. 19-20 *Setting data and chromatogram images*

Once the chromatogram is obtained, the detected peaks must be interpreted. These are identified according to the Relative Retention Time (RRT), which is compared to the Retention Time (RT) of the well-known substance in the standard. The reference substance originates from the laboratory's internal bibliography.

$$RRT = \frac{aRT\ DTC_{peak}}{aRT\ STD_{peack}}$$

Where:

aRT DT_{peak} is the Absolute Retention Time of peak detected.

aRT STD_{peak} is the Absolute Retention Time of peak of the standard.

After identifying the VOCs in the chromatogram, the concentration can be calculated. The peak area values are entered into a spreadsheet, where there are also the Response Factor (RF) values for each substance. In addition, the volume of air extracted during sampling must be entered.

The concentration of the identified substances can be calculated with the following equation (1).

$$C = \frac{RF \cdot A \cdot DN \cdot Ve}{Nlt} \quad [\text{mg/Nm}^3] \qquad (1)$$

Where:

RF is the Response Factor.

A is the peak area.

DN is the dilution number.

Ve is the volume of extraction solution.

Nlt is the value of normalized Liters.

The same methodology of analysis has been also applied to the samples taken from the workplace areas (with Radiello). In this case, as well, the passive samples are carbon adsorbent vials. The sampling during the 8 hours of work, allows solvent adsorption from the air.

7.2.1. SAMPLING RESULTS

This section reports the results of the analysis of the collected samples.

They refer to indoor tests in the working environment and outdoor tests in the abatement system.

7.2.1.1. Outdoor

The average amount of CO, NOx and PM emission out is reported in the following table 2, these values are referred to each sample campaign. As mentioned above, during the year 2020 only one sampling session for each season could be carried out due to restrictions from Co-Vid19.

	FEBRUARY 2020	**DECEMBER 2020**	**APRIL 2021**	**JULY 2021**	**SEPTEMBER 2021**	**DECEMBER 2021**
	[mg/Nm^3]	[mg/Nm^3]	[mg/Nm^3]	[mg/Nm^3]	[mg/Nm^3]	[mg/Nm^3]
CO	26.1	30.8	38.4	32.1	39.3	60.5
NO_x	5.7	7.0	8.2	7.1	8.6	12.8
PM	0.27	0.27	0.28	0.31	0.32	0.45

Tab. 2 *Average amount of CO, NOx, and PM out from RTO*

The following tables (Table 3, 4, 5) show the VOCs identified and their concentrations in mg referred to Nm^3 of total air in the inlet flow.

	FEBRUARY 2020			**DECEMBER 2020**		
VOC	Point 1 IN SCRUBBER [mg/Nm^3]	Point 2 IN RTO [mg/Nm^3]	Point 3 OUT RTO [mg/Nm^3]	Point 1 IN SCRUBBER [mg/Nm^3]	Point 2 IN RTO [mg/Nm^3]	Point 3 OUT RTO [mg/Nm^3]
Ethylbenzene	22.9	11.6	0.3	12.7	6.8	0.4
Methanol	0.0	0.0	0.0	0.0	0.0	0.0
MIBK	83.4	65.8	0.8	73.3	51.7	0.4
N-Hexane	0.0	0.0	0.0	0.0	0.0	0.0
Styrene	54.3	23.6	0.0	65.8	32.8	0.0
I-Butyl Acetate	92.9	67.7	0.0	84.1	61.9	0.0
MEK	86.8	54.2	0.0	99.7	64.7	0.0
Methyl Acetate	8.4	5.5	0.0	5.9	3.9	0.0
N-Butyl Acetate	98.7	78.6	0.7	67.3	54.2	0.8
Propyl Acetate	2.9	1.9	0.0	2.1	0.9	0.0
Toluene	257.4	186.3	0.9	296.1	201.2	0.7
M-Xylene	12.2	5.4	1.0	44.3	19.8	1.2
O-Xylene	20.2	12.7	0.3	46.7	33.6	0.7
Acetone	369.2	253.1	9.4	457.4	364.5	7.9
Ethanol	116.2	79.1	0.8	127.6	86.6	0.6
Ethyl Acetate	74.4	44.2	0.0	89.1	48.9	0.0
N-Heptane & Is.	0.0	0.0	4.7	0.0	0.0	5.5
N-Pentane	0.0	0.0	0.6	0.0	0.0	0.7
PMA	8.4	4.3	0.0	6.3	4.1	0.0
TOTAL [mg/Nm^3]	1308.3	894.0	19.5	1478.4	1035.6	18.9

Tab. 3 *Sample campaigns during 2020*

	APRYL 2021			**JULY 2021**		
VOC	Point 1	Point 2	Point 3	Point 1	Point 2	Point 3

	IN SCRUBBER [mg/Nm^3]	IN RTO [mg/Nm^3]	OUT RTO [mg/Nm^3]	IN SCRUBBER [mg/Nm^3]	IN RTO [mg/Nm^3]	OUT RTO [mg/Nm^3]
Ethylbenzene	53.2	23.3	0.6	33.6	19.6	0.5
Methanol	0.0	0.0	0.0	0.0	0.0	0.0
MIBK	92.2	69.6	1.3	88.5	30.1	1.3
N-Hexane	0.0	0.0	0.0	0.0	0.0	0.0
Styrene	80.1	74.4	0.0	80.1	66.7	0.0
I-Butyl Acetate	83.7	56.3	0.0	75.1	47.4	0.0
MEK	101.7	93.9	0.0	106.8	87.9	0.0
Methyl Acetate	7.2	5.3	0.0	6.8	4.2	0.0
N-Butyl Acetate	136.2	122.2	0.9	118.7	102.3	0.9
Propyl Acetate	1.9	1.0	0.0	2.9	2.1	0.0
Toluene	345.7	278.1	0.4	333.6	242.1	0.6
M-Xylene	66.7	34.7	1.4	87.7	41.6	1.3
O-Xylene	89.9	79.5	0.5	74.9	68.5	0.6
Acetone	522.9	488.1	8.2	430.0	388.3	8.2
Ethanol	149.9	102.8	0.9	142.3	97.1	0.7
Ethyl Acetate	105.5	68.3	0.0	88.8	51.2	0.0
N-Heptane & Is.	0.0	0.0	5.2	0.0	0.0	6.6
N-Pentane	0.0	0.0	0.8	0.0	0.0	0.7
PMA	6.9	4.9	0.0	8.6	5.2	0.0
TOTAL [mg/Nm^3]	1843.7	1502.4	20.2	1678.4	1254.3	21.4

	SEPTEMBER 2021			**DECEMBER 2021**		
VOC	Point 1 IN SCRUBBER [mg/Nm^3]	Point 2 IN RTO [mg/Nm^3]	Point 3 OUT RTO [mg/Nm^3]	Point 1 IN SCRUBBER [mg/Nm^3]	Point 2 IN RTO [mg/Nm^3]	Point 3 OUT RTO [mg/Nm^3]
Ethylbenzene	44.1	22.5	0.7	60.8	47.8	0.8
Methanol	0.0	0.0	0.0	0.0	0.0	0.0
MIBK	74.6	61.6	1.3	96.3	70.2	1.3
N-Hexane	0.0	0.0	0.0	0.0	0.0	0.0
Styrene	80.1	61.5	0.0	80.1	60.3	0.0
I-Butyl Acetate	67.6	39.6	0.0	94.5	70.2	0.0
MEK	113.3	91.2	0.0	149.2	112.6	0.0
Methyl Acetate	6.8	5.1	0.0	6.8	5.3	0.0
N-Butyl Acetate	98.3	85.3	1.0	144.8	129.9	1.3
Propyl Acetate	2.9	2.3	0.0	3.0	2.5	0.0
Toluene	369.7	278.4	0.8	433.2	384.7	1.1
M-Xylene	97.9	55.7	1.1	111.3	67.7	1.6
O-Xylene	66.6	51.2	0.6	104.2	90.0	0.8
Acetone	576.5	484.5	8.2	660.4	503.7	8.2
Ethanol	151.5	108.2	0.6	174.7	115.9	0.5
Ethyl Acetate	91.3	68.8	0.0	110.1	87.1	0.0
N-Heptane & Is.	0.0	0.0	6.5	0.0	0.0	7.6

N-Pentane	0.0	0.0	0.6	0.0	0.0	0.9
PMA	8.3	5.0	0.0	10.0	7,3	0.0
TOTAL [mg/Nm^3]	1849.5	1420.9	21.4	2239.4	1747.9	24.1

Tab. 4-5 *Sample sessions during 2021*

Table 6 shows the concentration for each VOC in the inlet and outlet flows as an average of all sampling campaigns. These quantities refer to the "gross value", namely before passing through the wet scrubber. In fact, it can be noted that after running through this system, there is a clear reduction in the concentration of VOCs due to the adsorption of some of them in the water (mainly the acetone) and the filtration of the sanding dust containing them. Therefore, as can be seen, the "gross value" of 1.7 g/Nm^3 is higher than the minimum required for the thermal oxidiser's self-sustaining mode (greater than 1.5 g/Nm^3). However, in practice there are several periods of the year when this minimum threshold is not reached in the inlet flow to the RTO, as shown in previously tables. This causes a continuous need of methane to properly feed the combustion chamber.

VOC	AVERAGE INLET FLOW IN PRE-SCRUBBER [mg/Nm^3]	AVERAGE OUTLET FLOW FROM RTO [mg/Nm^3]
Ethylbenzene	37.9	0.6
Methanol	0.0	0.0
MIBK	84.7	1.0
N-Hexane	0.0	0.0
Styrene	73.4	0.0
I-Butyl Acetate	83.0	0.0
MEK	109.6	0.0
Methyl Acetate	7.0	0.0
N-Butyl Acetate	110.7	0.9
Propyl Acetate	2.6	0.0
Toluene	339.3	0.8
M-Xylene	70.0	1.3
O-Xylene	67.1	0.6
Acetone	502.7	8.3

Ethanol	143.7	0.7
Ethyl Acetate	93.2	0.0
N-Heptane & Is.	0.0	6.0
N-Pentane	0.0	0.7
PMA	8.1	0.0
TOTAL [mg/Nm^3]	**1733.0**	**20.9**

Tab. 6 *Average concentration of VOCs in sample campaigns*

Furthermore, the Tab. 7 shows the VOCs abatement performance values for each measurement campaign.

	FEBRUARY 2020	DECEMBER 2020	APRIL 2021	JULY 2021	SEPTEMBER 2021	DECEMBER 2021
Purification Yield [%]	**98.51**	**98.72**	**98.90**	**98.73**	**98.84**	**98.93**

Tab. 7 *Yield % of VOCs abatement for each campaign*

The purification efficiencies obtained are in line with the performance of RTOs, as expected (Cao & Lee, 2023; Lewandowski, 2017; Pu et al., 2021).

7.2.1.2. Indoor

In the following table 8 are shown the sum of VOCs amount detected in the two departments of the company, where solvents are used.

	Sampling periods						**EXPOSURE LIMIT VALUES [mg/Nm^3]**			
	Feb 20	Dec 20	Apr 21	Jul 21	Sep 21	Dec 21	**T.L.V. (ACGIH)**		**All. XXXVIII D.Lgs. 81/08**	
VOC	**Concentration [mg/Nm^3]**						T.W.A	STEL	8 hours	Short time*
Acetone	2.9	3.5	1.8	2.5	0.8	4.6	1187	1781	1210	-
MEK	0.3	0.2	0.4	0.3	0.5	0.6	590	885	600	900
Ethyl Acetate	0.6	1.1	1.2	0.9	3.6	2.6	1441	-	-	-
MIBK	2.0	2.6	1.0	0.3	0.5	1.7	82	307	83	208
Toluene	0.7	1.2	1.8	0.6	1.4	2.5	75.4	-	192	-
Isobutyl Acetate	2.7	2.3	1.7	0.4	0.8	2.7	713	-	-	-
N-Butyl Acetate	3.3	0.4	5.6	0.8	3.2	6.5	713	950	-	-
Ethylbenzene	0.4	1.4	0.5	0.2	0.8	1.3	87	-	442	884

M-Xylen	1.1	0.5	1.8	0.4	2.5	4.0	434	651	221	442
O-Xylen	0.3	0.7	0.5	0.1	0.1	1.0	434	651	221	442
TOTAL	**14.3**	**13.9**	**16.3**	**6.5**	**14.2**	**27.5**				

*15 minutes max.

Tab. 8 *VOCs concentration in workplaces*

The exposure limit values definition is explained below.

- TLV-TWA is the time-weighted average concentration, over a conventional 8-hour working day and 40 hours per week, to which almost all workers can be repeatedly exposed without adverse effects. Value proposed by the ACGIH-American Council of Government Industrial Hygienists.
- TLV-STEL is the threshold limit value for a short exposure time. Namely the TWA concentration in 15 minutes that must not be exceeded at any time during the working day even if the 8-hour TWA does not exceed the TLV-TWA. The TLV-STEL is the concentration that it is assumed that workers can be exposed to continuously for a short period of time without suffering irritation effects, chronic or irreversible tissue damage, toxic dose response effects, or materially reduce work efficiency.

8. THEORETICAL PHASE

During this PhD experience, there was a cooperation with the Department of Materials and Chemical Engineering at Polytechnic of Milan. During this experience it was possible to use their GasDs kinetic model to study the preliminarily behavior of the proposed system. The GasDs software was used to perform the kinetic analysis of the combustion of biomass and VOCs in a single reaction volume. The data collected from the experimental analyses were used as a base line. This theoretical study aims to demonstrate the compatibility between the recovery of waste raw material and pollutant abatement. It also aims to provide starting values for abatement and energy recovery efficiencies.

8.1. GasDs – KINETIC PACKAGE FOR SIMULATIONS

To model thermochemical processes of combustion is clearly a big challenge.
The development of these types of models is complex due to the variety of elements involved and the multiphase and multi-scale nature of the conversion process of the solid fuel (Mettler et al., 2012). As mentioned in (Ranzi et al., 2016), its complexity occurs at several levels:

- Multicomponent problem: usually the solid fuels are a complex mixture of inorganic and organic species.
- Multiphase problem: the first reaction involves solid materials and generates solid, liquid and gas phase components. Then, the secondary reaction products, which take place in a multicomponent gas phase, involves heterogeneous gas-solid reactions.
- Multiscale problem: the transport phenomena in the gas and solid phase and between the solid and gas phases need to be considered at both the particle and the reactor scale to characterize their relative role with respect of chemical kinetics.

The GasDs kinetic-based package used, is particularly suited to evaluate the pyrolysis, gasification, and combustion of biomass. This dynamic model was already introduced and validated on biomass (Ranzi et al., 2014). It has a detailed kinetic scheme and several scales: particle, reactor layer.

The model is introduced and described very well in the paper by (Cabianca et al., 2016). As well as are indicated the transformations involved and the discretization processes in the radial and longitudinal direction. The latter approximate the reactor to a continuous series of layers where the conditions for the gas phase are assumed homogeneous. While the biomass particles are discretized into multiple concentric layers. The approximation to reduce the dynamic process described by a Partial Differential Equations (PDEs) to an Ordinary Differential Equations system (ODEs), is managed through advanced numerical methods (Buzzi-Ferraris & Manenti, 2012). The preliminary operation to data input is the CHNSO analysis, i.e. the characterisation of the solid part in terms of Carbon, Hydrogen, Nitrogen, Sulphur and Oxygen. This is dependent on the substrate type to be simulated, in the present case virgin wood biomass. Then the lignin components (LIG-O, LIG-H and LIG-C) must be entered in kmol of C, H, O. The spreadsheet provides these values in terms of the final equivalent composition in percentage and these parameters must be set in GasDs.

After the CHNSO analysis, the input parameters must be set in a series of spreadsheets with several specific sections to be compiled.

- Component List: selection of the appropriate components from solid and gas spreadsheets.
- Gas-Solid Reaction List: selection of the appropriate reactions to be modelled from kinetic spreadsheet.
- Particle characterization: number, number of particle sectors, initial temperature, uniform initial temperature.

- Reactor Geometry: cylindrical, number of volume elements.
- Gaseous Agent Properties: selection of the flowrate, the start-up temperature for the gaseous agent and the composition (v/v%).
- Solid Composition: data input from the CHNSO analysis.
- Solid Feedstock data: selection of the flowrate and temperature.

When designing the simulation, special attention must be directed to the correct choice of the number of reaction volumes to be evaluated. This means that:

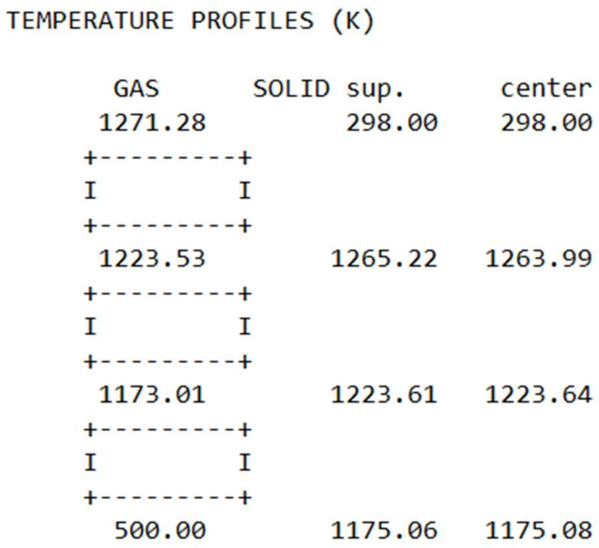
- 1 volume for quick is for approximate estimation.
- 2 volumes are for a real estimate of the reactor with good precision.
- 3 volumes are for very high precision.

The GasDs software returns output data on the concentrations of the most important gaseous chemical species, as can be seen in the table 9. These chemical species are the more representative of the phenomenon to be explored. In addition, they are extremely significant for the environmental protection.

GAS OUTPUT [μg/h]	
H_2	Hydrogen
H_2O	Water vapour
CO	Carbon Monoxide
CO_2	Carbon Dioxide
CH_4	Methane
C_3H_6	Propylene
C_3H_8	Propane
C_2H_2	Acetylene
C_2H_4	Ethylene
C_2H_6	Ethane
CH_2O	Formaldehyde
CH_3OH	Methanol
HCOOH	Formic Acid
C_7H_8	Toluene
C_2H_6O	Methylene

Tab. 9 *Gaseous species output from GasDs*

The temperature profile is shown for the gas and solid phase in each reactor sector, as shown in the following figure XX from the output sheet. The mass transfer models accurately predict the overheating of the particle core in case of large Dp (combustion heat trapped in the core due to poor heat transfer).



```
TEMPERATURE PROFILES (K)

          GAS      SOLID sup.      center
        1271.28          298.00    298.00
       +---------+
       I         I
       +---------+
        1223.53         1265.22   1263.99
       +---------+
       I         I
       +---------+
        1173.01         1223.61   1223.64
       +---------+
       I         I
       +---------+
         500.00         1175.06   1175.08
```

Fig. 21 *Example of output temperature profiles from GasDs*

8.1.1. CALCULATION TIME

As previously mentioned, the accuracy is proportional to the number of reactor volumes. On the other hand, there is a large increase in the calculation time.

For this research, the simulation of one volume has been done in the early stages of the studies to test the compatibility between the biomass and the VOCs, i.e. to verify the correct input baseline for the combustion start-up. In this case the calculation time is about 2-4 hours in average for each simulation.

Subsequently have been chosen two reactor volumes, with an average calculation time of about 6-8 hours per simulation.

8.2. IMPUT DATA

To achieve reasonable simulations, some sampling results and some real characteristics were taken as basic data. With regard of solvents were used the most representative ones (Acetone, Toluene, Ethanol etc.), since the GasDs simulation package does not include all types. Their quantities are representative of the average found in the samples taken and the painting composition used. In the Table 10 are shown these values and the types of VOCs considered. The total concentration is 1.3 g/Nm^3, lower than what would be required for an RTO to be self-sustaining, but it is representative of common situations. Exactly those that cause a high methane consumption problem for the operation of the thermal oxidizer.

Regarding biomass, two kinds were considered, virgin softwood and virgin hardwood, as representative of biomass used in the production of furniture and fixtures. In GasDs is needed to use the reference unit LIG–C, LIG-O and LIG-H to perform the biomass type. To obtain these reference units, it is essential to know the elemental composition of the lignin of the wood species. (Faravelli et al., 2010) have been proposed the elemental analysis of different lignin and have been reached the equivalent composition in terms of "reference components". Specifically, the LIG-C, with the largest amount of carbon, is representative of softwood. On the other hand, LIG–O and LIG–H, that are richest in O and H respectively, are more representative of the structures of hardwood.

The elemental composition has been used to perform the CHNSO analysis and achieve the feedstock composition as can be observed in Tab. 12.

VOC	Chemical formula	Amount [mg/Nm^3]
Acetone	C_3H_6	500
Toluene	C_7H_8	350
MEK	C_4H_8O	150
Xylenes	C_8H_{10}	150

Ethanol	C_2H_6O	150
	Total	**1300**

Table 10 *VOCs amount input data*

	REACTOR GEOMETRY **CYLINDRICAL**	
	Case 1	Case 2
Radius [m]	**0.55**	**0.80**
High [m]	**1.0**	**2.0**
Volume [m^3]	**1.0**	**4.0**

Tab. 11 *Reactor volume geometry*

	HARDWOOD	**SOFTWOOD**
LIG -O	20 %	10 %
LIG-C	30 %	60 %
LIG-H	50 %	30 %

Tab. 12 *Reference component of biomass*

The operating time of the proposed system was assumed to be 8 hours, which corresponds to a typical working day. In addition, all proposed simulations are referred to the 'day 1', i.e. the first day when the system first comes into use. In Table 13 are shown the type of wood, reactor volume and pollutant air feed chosen.

SOFTWOOD			**HARDWOOD**		
BIOMASS FEED	REACTOR VOLUME	VOCs + AIR FEED	BIOMASS FEED	REACTOR VOLUME	VOCs + AIR FEED
[kg/h]	[m^3]	[Nm^3/h]	[kg/h]	[m^3]	[Nm^3/h]
2.5	1	1000	2.5	1	1000
		5000			5000
	4	1000		4	1000
		5000			5000
10	1	1000	10	1	1000
		5000			5000
	4	1000		4	1000
		5000			5000

Tab. *13* *Type of wood, biomass quantity, reactor volume and Air+VOCs feed*

In regard of the internal reactor temperature, a range of 1023-1123 K was considered (Tab. 14). This choice was made to study solvent abatement in the temperature range where self-ignition of the mixture occurs as well as in the thermal oxidizer. Therefore, a Δt = 20 K was chosen to evaluate the abatement efficiency trend as the temperature increase in the reaction chamber. Each temperature scenario that is assumed refers to the maintenance of that T value during the entire runtime.

TEMPERATURE [K]					
1023	1043	1063	1083	1103	1123

Tab. 14 *Temperature steps*

The simulations are named by highlighting the main parameters. For example, "HW_VOC_1000_2.5_1" means that are considered: Hardwood, AIR+VOC feed of 1000 Nm^3/h, biomass amount of 2.5 kg/h and reactor volume of 1 m^3.

The following table 15 summarises the eight simulated scenarios for both softwood and hardwood. Each scenario, as already described, was also simulated for every temperature increment (1023 – 1043 – 1063 – 1083 – 1103 – 1123 K). The following table shows the titles of the simulations performed.

Hardwood simulation	Softwood simulation
HW_VOC_1000_2.5_1	SW_VOC_1000_2.5_1
HW_VOC_1000_2.5_4	SW_VOC_1000_2.5_4
HW_VOC_1000_10_1	SW_VOC_1000_10_1
HW_VOC_1000_10_4	SW_VOC_1000_10_4
HW_VOC_5000_2.5_1	SW_VOC_5000_2.5_1
HW_VOC_5000_2.5_4	SW_VOC_5000_2.5_4
HW_VOC_5000_10_1	SW_VOC_5000_10_1
HW_VOC_5000_10_4	SW_VOC_5000_10_4

Tab. 15 *Titles of simulation sets*

9. FINDINGS

Due to the large number of data collected, only a few of them will be shown below. The others will be available in the appendix. However, all comments are valid to those not shown in this chapter, also for the softwood biomass.

9.1. VOCs ABATEMENT

The following tables 16, 17 and graphs 22, 23, present the concentration trends of the outgoing gaseous compounds for each temperature set for the simulation **HW_VOC_1000_2.5_1** and **SW_VOC_1000_2.5_1.**

It can be observed that the output compound concentration decreases with increasing the reactor temperature, except for Carbon Dioxide and Water Vapour. These compounds show a gradual minimum increase as the operating temperature increases.

HW_VOC_1000_2.5_1

T [K]	1023	1043	1063	1083	1103	1123
	Output [μg/h]	Output [μg/h]	Output [μg/h]	Output [μg/h]	Output [μg/h]	Output [μg/h]
H_2	3.58E+05	2.56E+05	1.77E+05	1.19E+05	7.80E+04	5.21E+04
H_2O	3.78E+09	3.79E+09	3.78E+09	3.77E+09	3.75E+09	3.72E+09
CO	1.35E+09	1.03E+09	7.42E+08	5.06E+08	3.32E+08	2.20E+08
CO_2	1.21E+10	1.26E+10	1.30E+10	1.34E+10	1.35E+10	1.36E+10
CH_4	1.56E+06	1.10E+06	7.59E+05	5.08E+05	3.34E+05	2.23E+05
C_3H_6	3.80E+04	3.40E+04	2.88E+04	2.24E+04	1.57E+04	1.03E+04
C_3H_8	4.27E-01	2.08E-01	9.37E-02	3.80E-02	1.38E-02	4.87E-03
C_2H_2	1.51E+06	1.19E+06	9.35E+05	7.28E+05	5.61E+05	4.31E+05
C_2H_4	2.66E+06	2.06E+06	1.57E+06	1.18E+06	8.72E+05	6.38E+05
C_2H_6	1.29E+04	6.94E+03	3.41E+03	1.52E+03	6.17E+02	2.48E+02
CH_2O	5.05E+06	3.76E+06	2.75E+06	1.96E+06	1.37E+06	9.66E+05
CH_3OH	2.68E+06	1.98E+06	1.41E+06	9.72E+05	6.53E+05	4.42E+05
HCOOH	3.99E+05	2.81E+05	1.96E+05	1.37E+05	9.51E+04	6.68E+04
C_7H_8	1.76E+07	1.31E+07	9.65E+06	7.04E+06	5.09E+06	3.69E+06
C_2H_6O	7.55E+05	5.47E+05	3.83E+05	2.59E+05	1.71E+05	1.15E+05

Tab. 16 *HW_VOC_1000_2.5_1 gas out for each T*

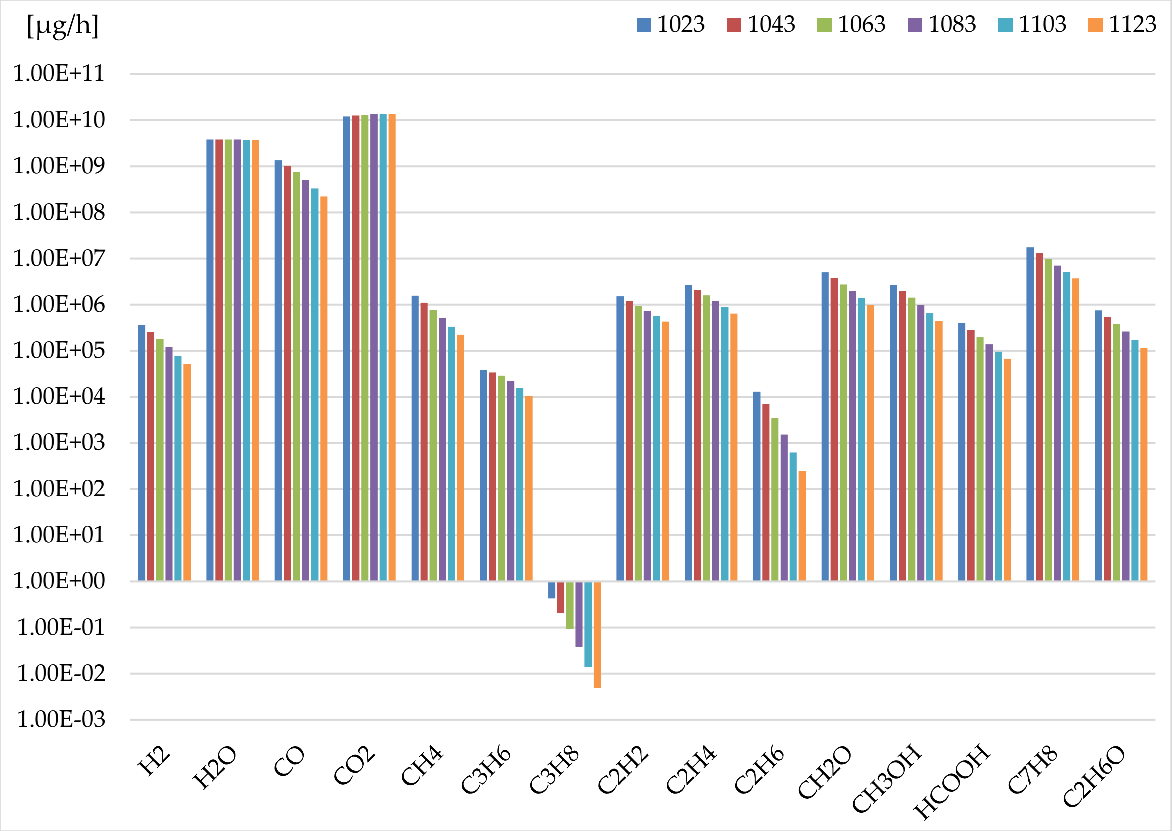


Fig. 22 *Trend of gas out for each T in HW_VOC_1000_2.5_1*

SW_VOC_1000_2.5_1

T [K]	**1023**	**1043**	**1063**	**1083**	**1103**	**1123**
	Output [µg/h]	Output [µg/h]	Output [µg/h]	Output [µg/h]	Output [µg/h]	Output [µg/h]
H_2	3.79E+05	2.69E+05	1.85E+05	1.23E+05	8.08E+04	5.42E+04
H_2O	3.73E+09	3.73E+09	3.73E+09	3.71E+09	3.69E+09	3.67E+09
CO	1.35E+09	1.02E+09	7.27E+08	4.92E+08	3.22E+08	2.14E+08
CO_2	1.23E+10	1.28E+10	1.32E+10	1.35E+10	1.37E+10	1.38E+10
CH_4	1.57E+06	1.11E+06	7.59E+05	5.06E+05	3.33E+05	2.23E+05
C_3H_6	3.89E+04	3.46E+04	2.91E+04	2.24E+04	1.56E+04	1.02E+04
C_3H_8	3.74E-01	1.82E-01	8.18E-02	3.29E-02	1.19E-02	4.22E-03
C_2H_2	1.50E+06	1.18E+06	9.21E+05	7.14E+05	5.48E+05	4.22E+05
C_2H_4	2.43E+06	1.87E+06	1.43E+06	1.07E+06	7.86E+05	5.76E+05
C_2H_6	1.22E+04	6.46E+03	3.14E+03	1.38E+03	5.56E+02	2.25E+02
CH_2O	4.83E+06	3.59E+06	2.61E+06	1.86E+06	1.30E+06	9.17E+05
CH_3OH	2.32E+06	1.71E+06	1.22E+06	8.39E+05	5.65E+05	3.85E+05
HCOOH	2.23E+05	1.56E+05	1.09E+05	7.59E+04	5.27E+04	3.72E+04
C_7H_8	1.70E+07	1.26E+07	9.31E+06	6.77E+06	4.89E+06	3.56E+06
C_2H_6O	7.35E+05	5.30E+05	3.69E+05	2.49E+05	1.64E+05	1.11E+05

Tab. 17 *SW_VOC_1000_2.5_1 gas out for each T*

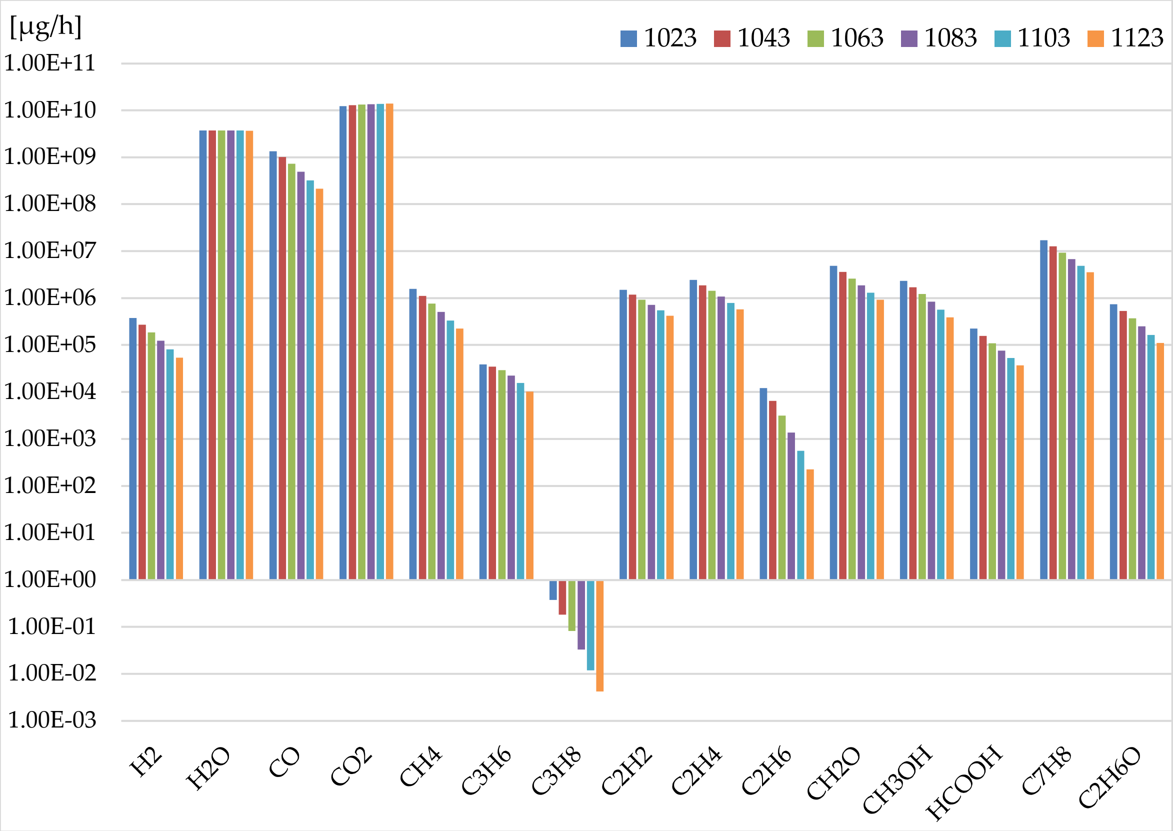


Fig. 23 *Trend of gas out for each T in SW_VOC_1000_2.5_1*

9.2. TRENDS IN OUTLET GAS CONCENTRATIONS AS A FUNCTION OF STEADY-STATE TEMPERATURES

The following graphs show the trend in the concentrations of each gaseous species at the outlet flow for each of the temperatures considered and for the eight Hardwood scenarios, as a representative case.

The function that most closely approximates the trend is a polynomial. Also, with this different presentation of the data, it can be observed that there is less emission of pollutants, as the operative temperature of the combustion chamber increases.

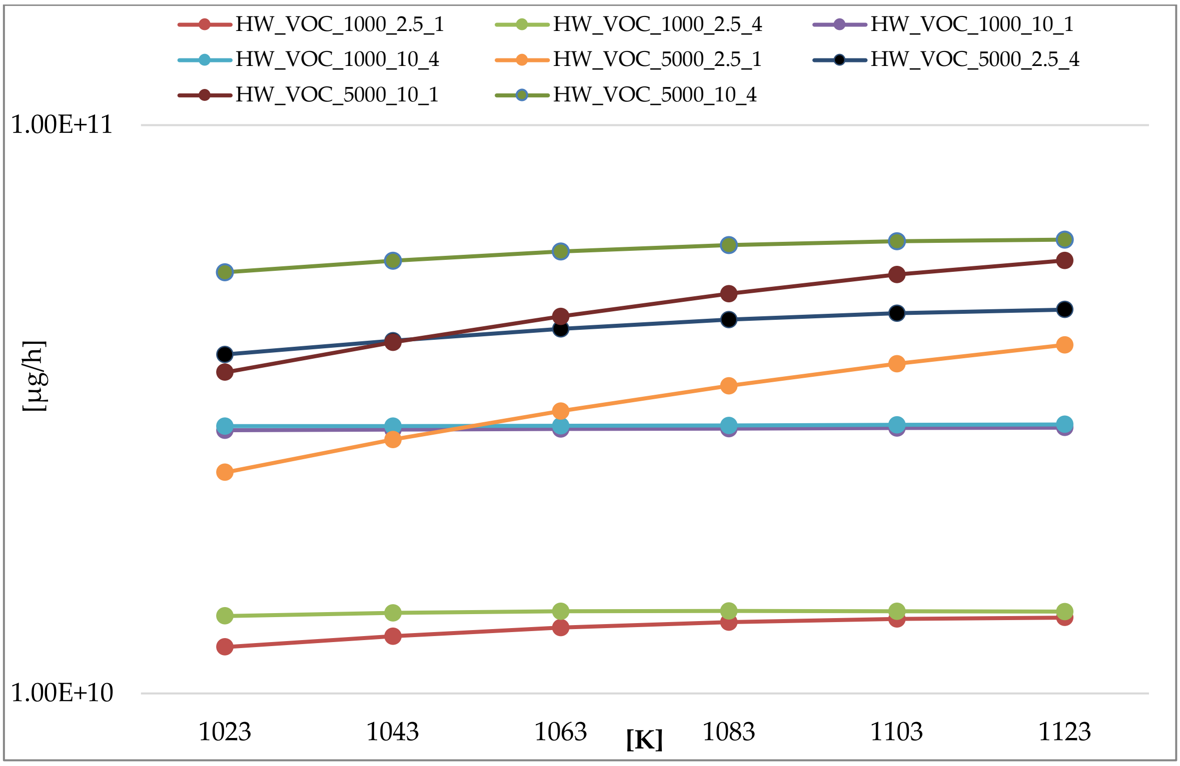


Fig. 24 *Carbon Dioxide*

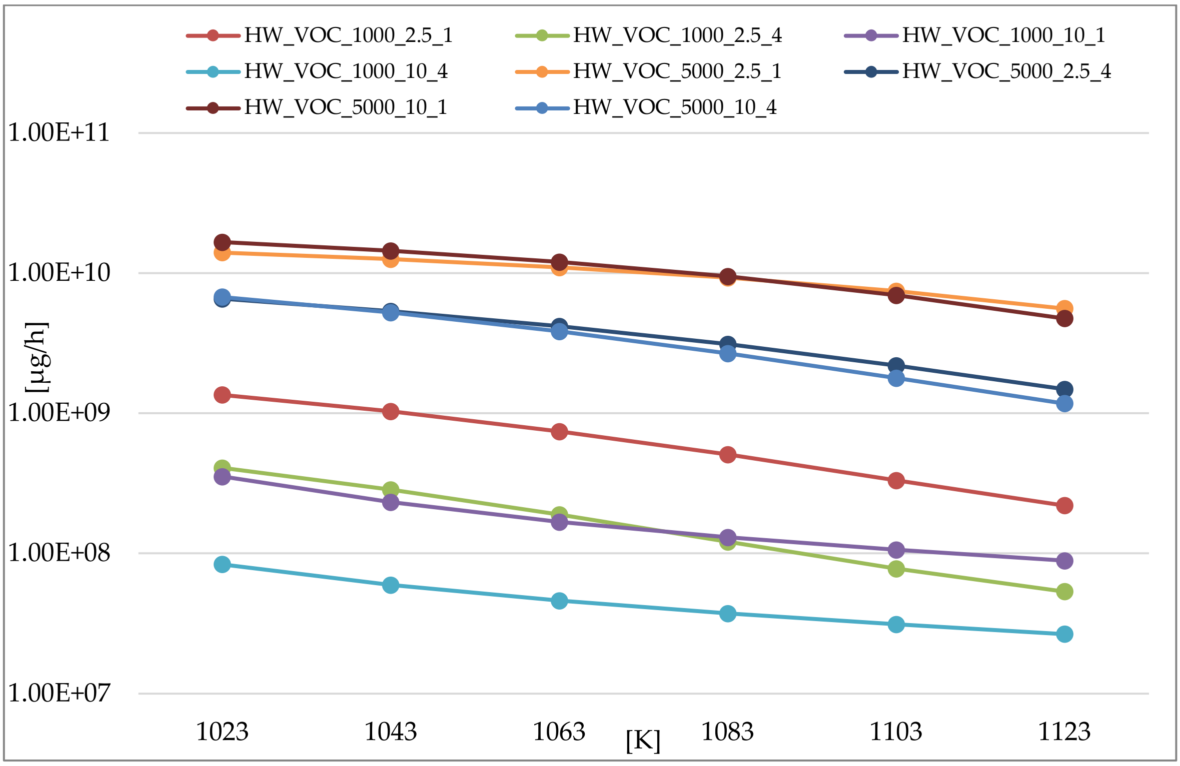


Fig. 25 *Carbon Monoxide*

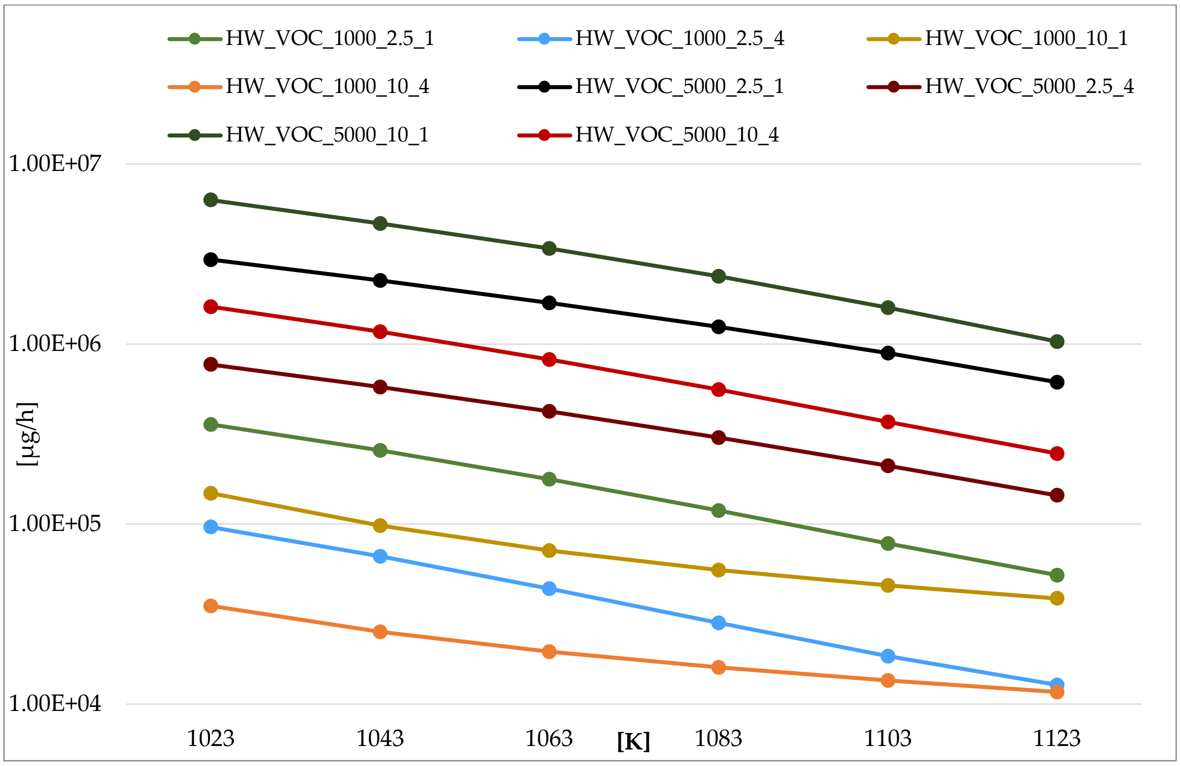


Fig. 26 *Hydrogen*

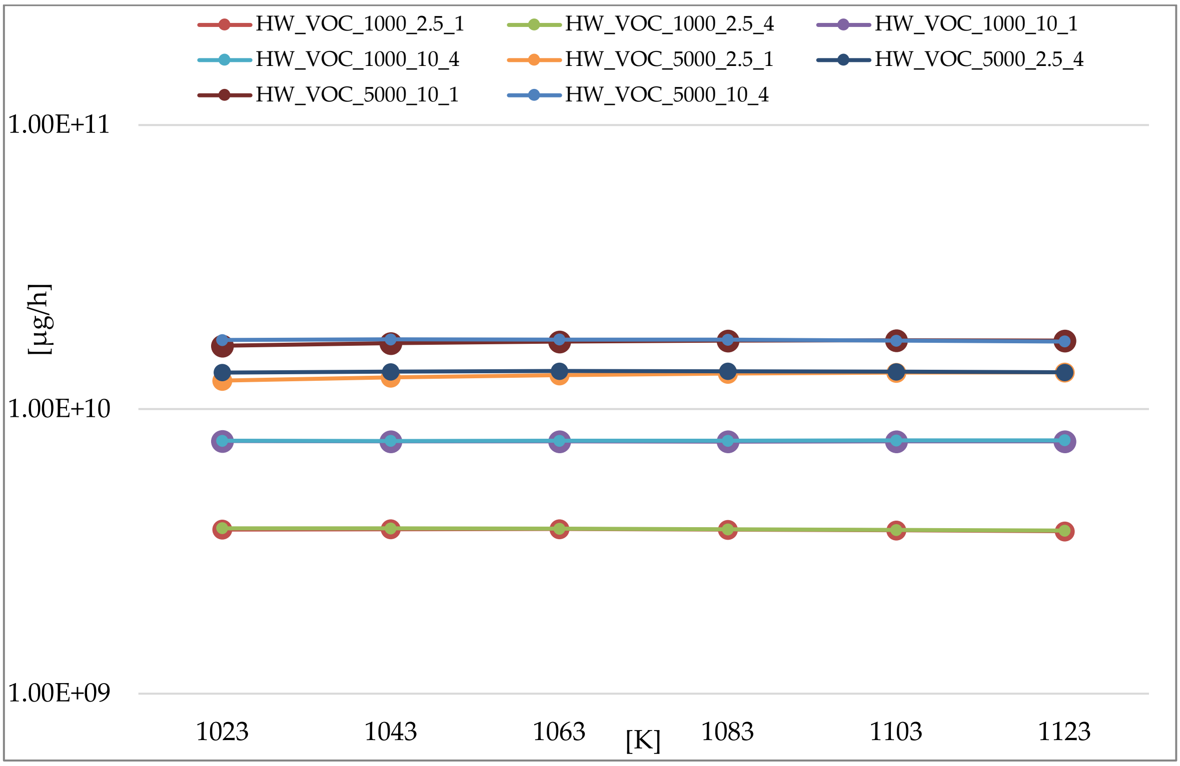


Fig. 27 *Water vapour*

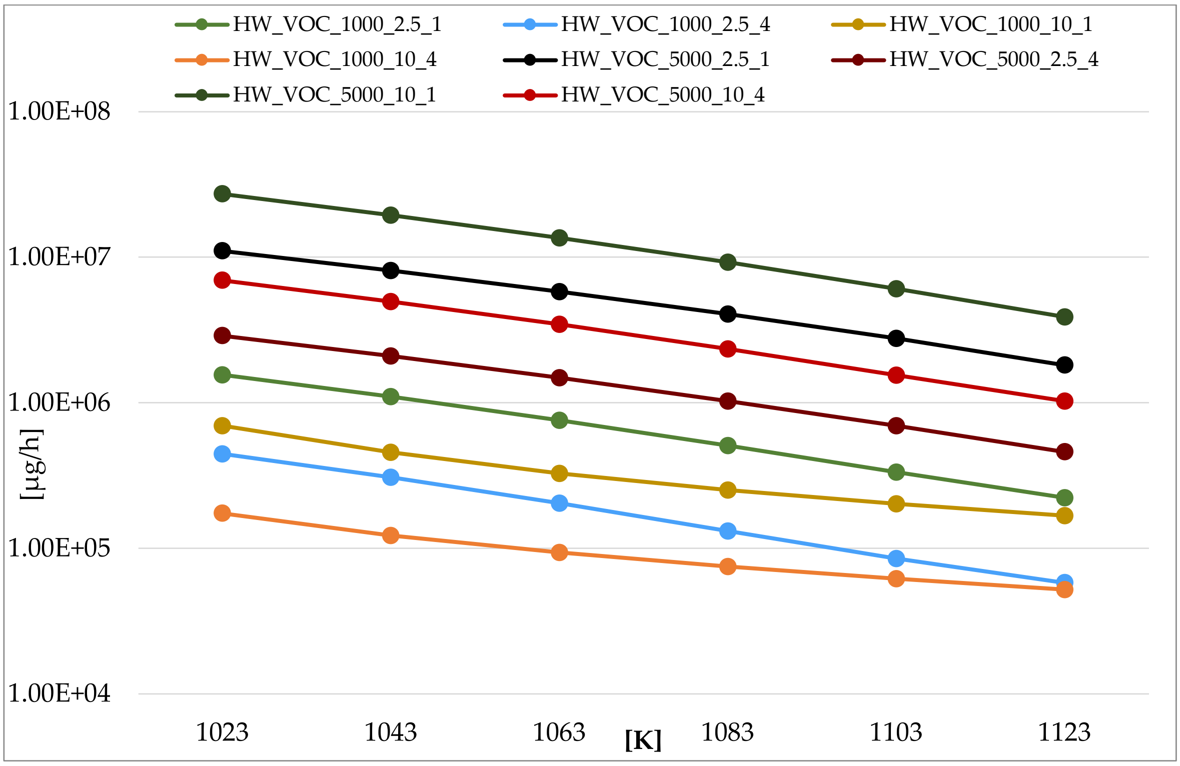


Fig. 28 *Methane*

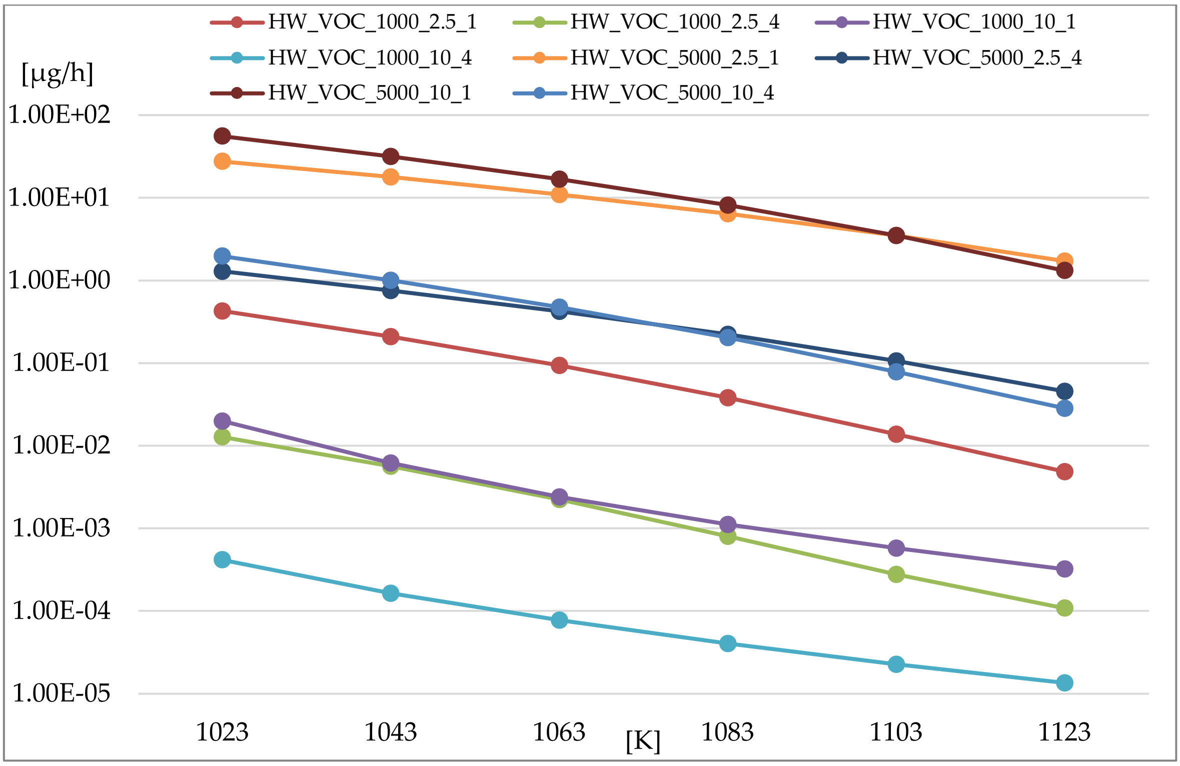


Fig. 29 *Propane*

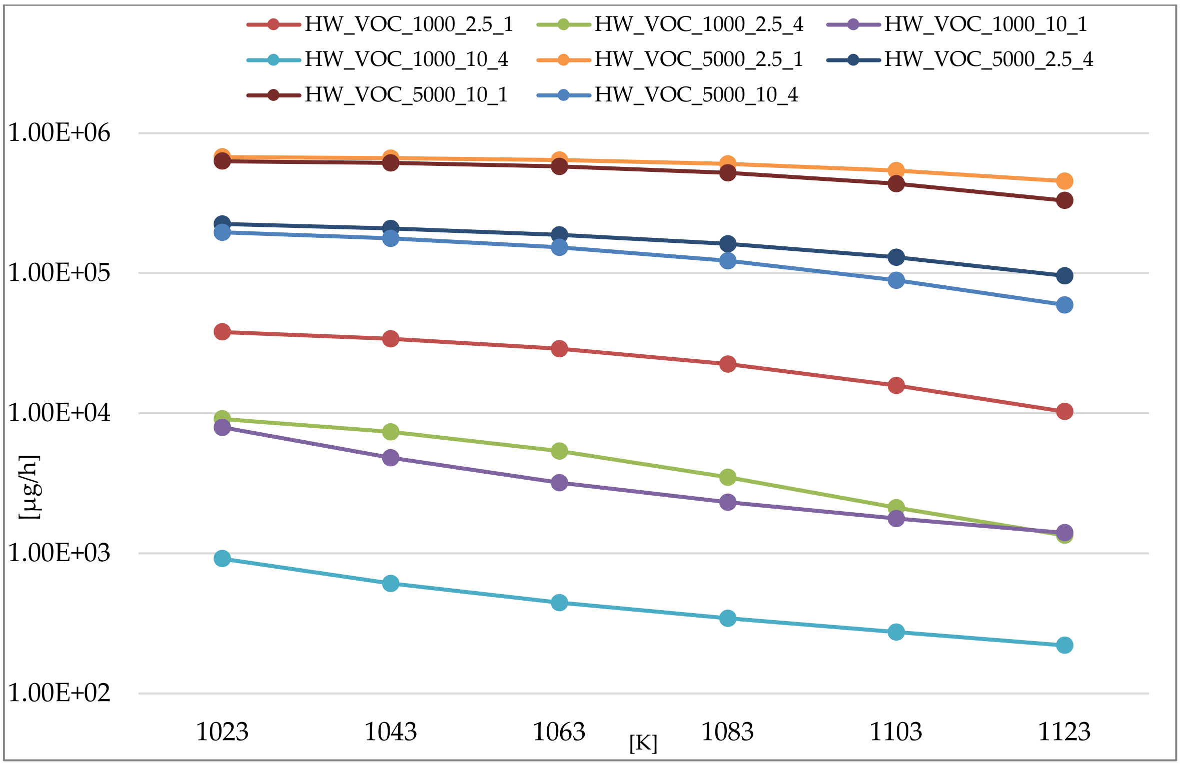


Fig. 30 *Propylene*

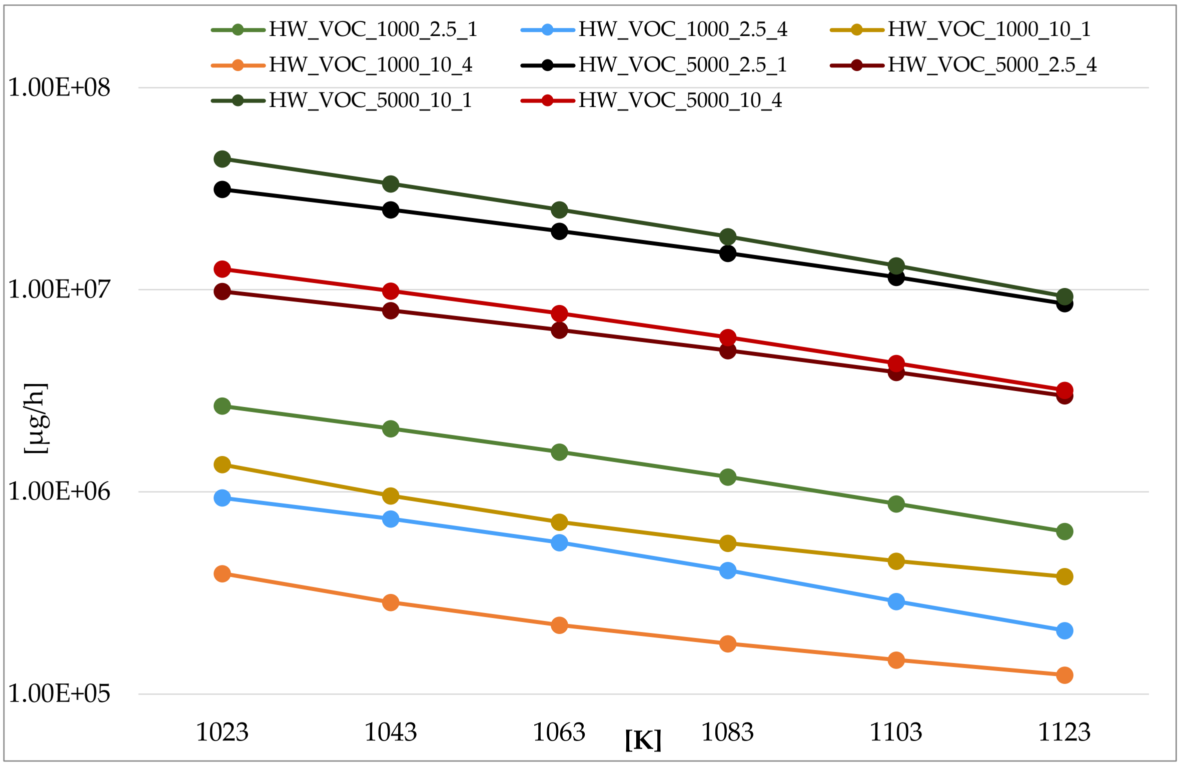


Fig. 31 *Ethylene*

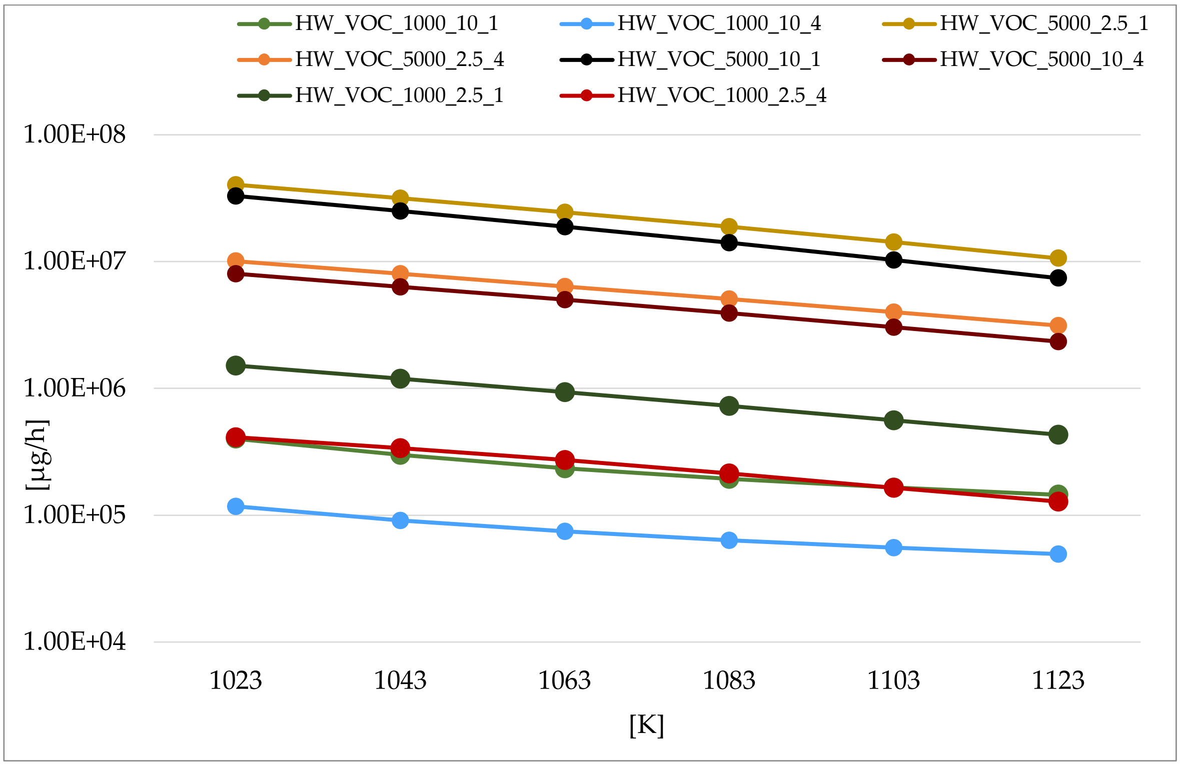


Fig. 32 *Acetylene*

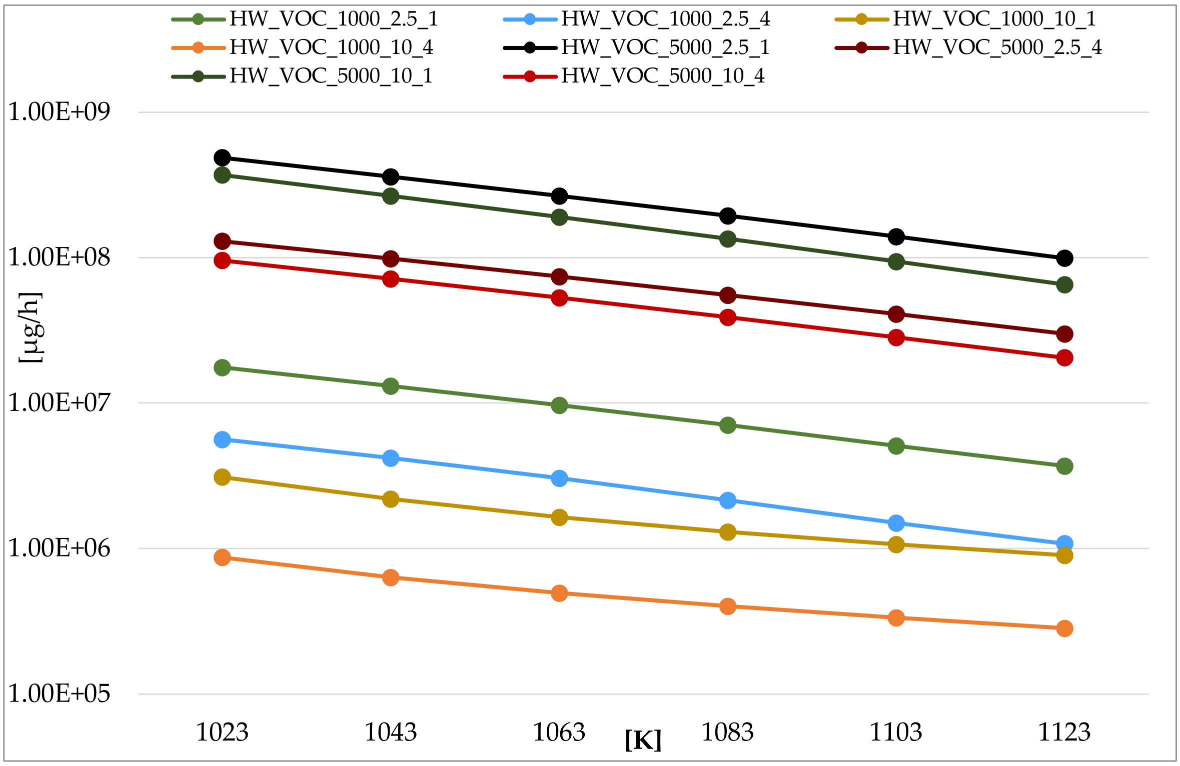


Fig. 33 *Toluene*

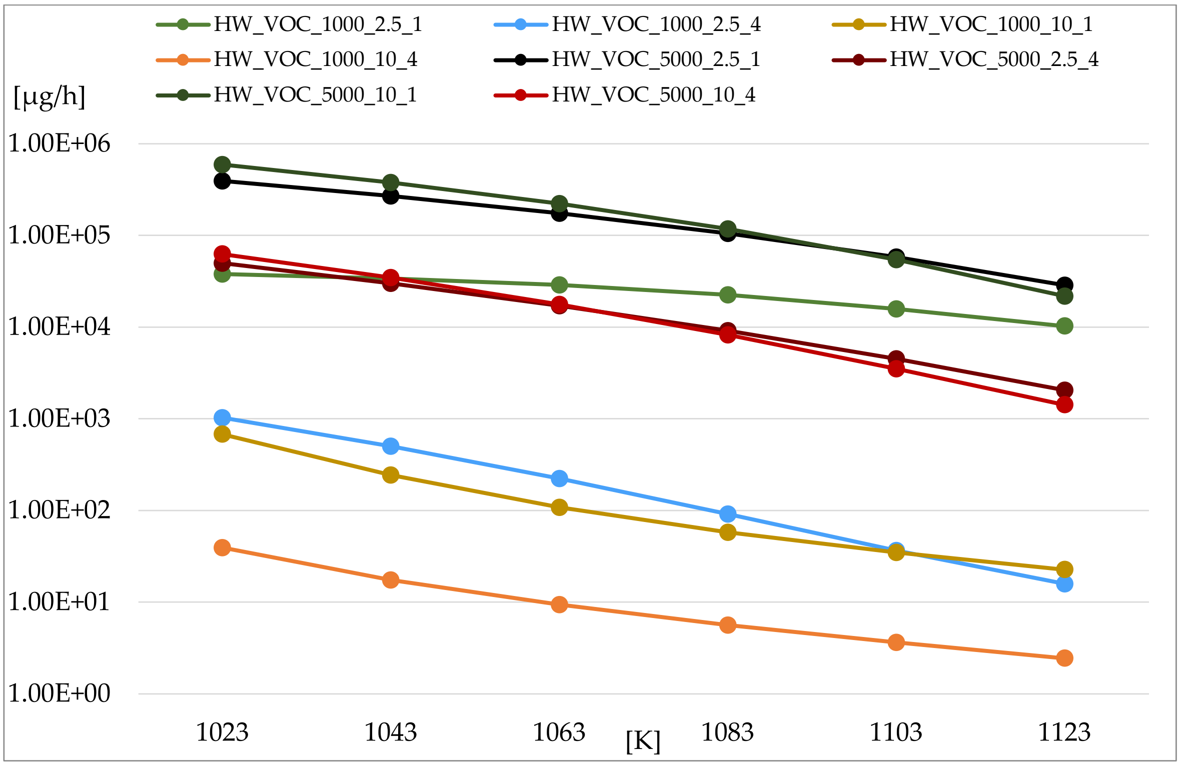


Fig. 34 *Ethene*

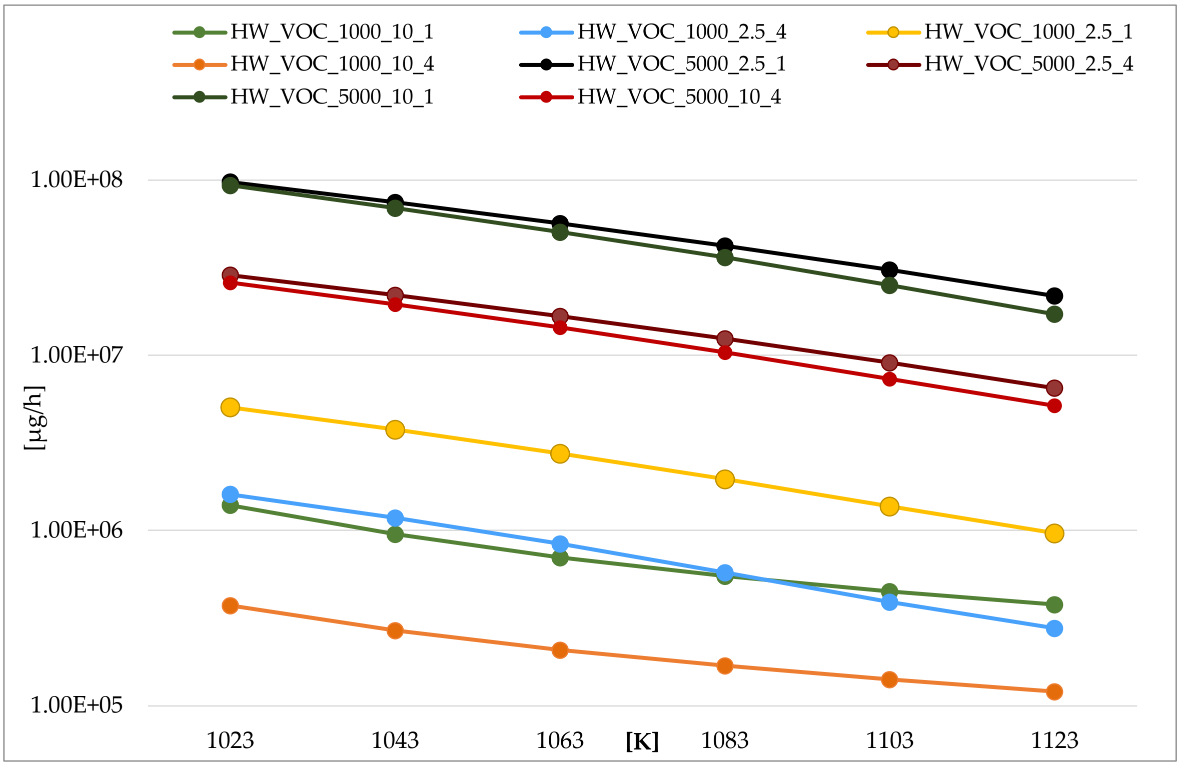


Fig. 35 *Formaldehyde*

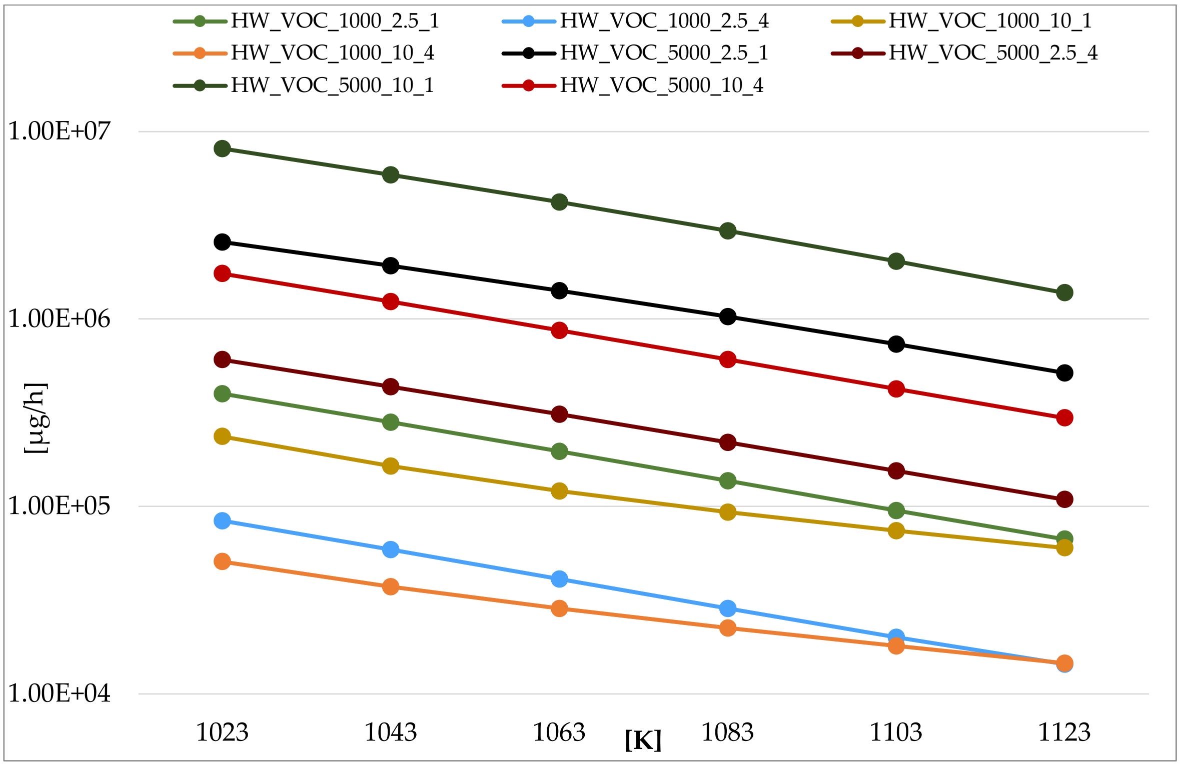


Fig. 36 *Formic Acid*

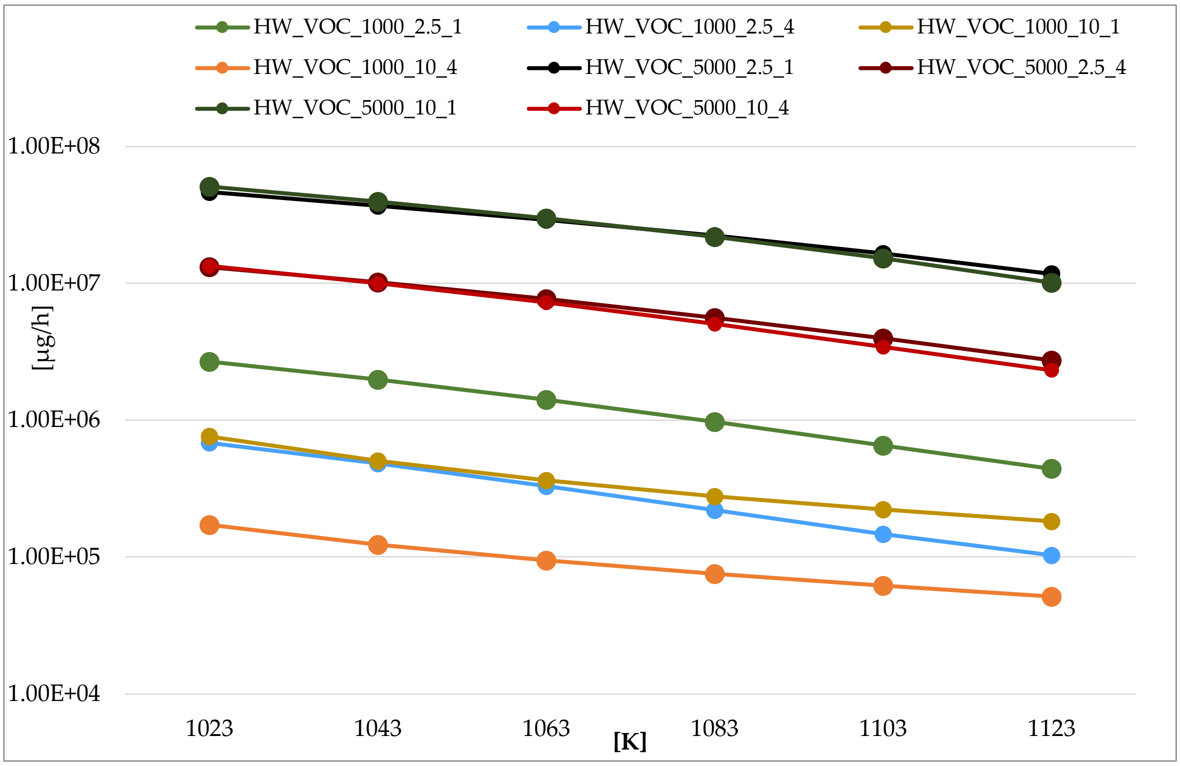


Fig. 37 *Methanol*

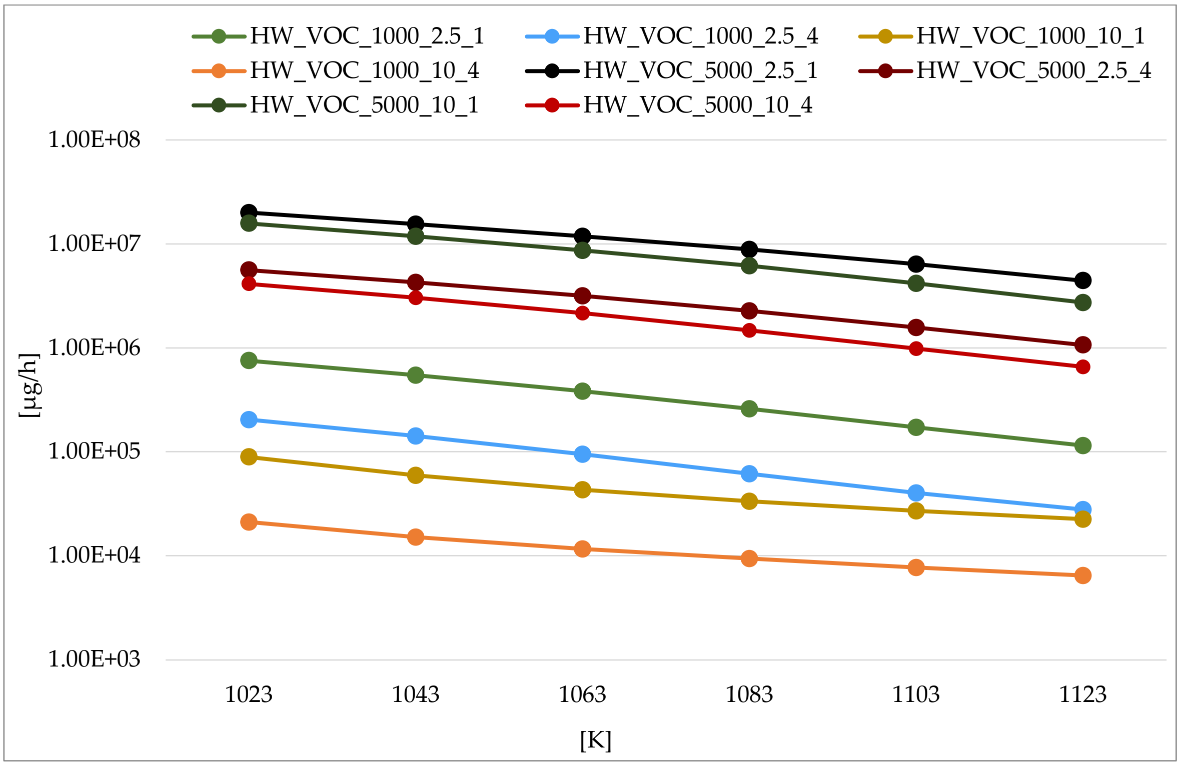


Fig. 38 *Ethanol*

9.3. VOCs AMOUNT DURING THE 8-HOUR WORKING DAY

The following graphs show the trends for the most important pollutants during the 8 hours of running, for the minimum and maximum temperatures of the range (1023 – 1123 K). The study aims to focus on the steady state regime when the temperature in the reaction chamber is maintained optimal (and constant) for the thermal destruction of VOCs and the complete biomass burning.

As can be observed from the trends, the initial phenomenon of rapid increase and change in amount is limited in time, within the first hour. This is caused by the start-up phase. After this period, there is a constant output flow of the compounds.

As a reference case the simulations are shown: HW_VOC_1000_2.5_1 and SW_VOC_1000_2.5_1.

HW_VOC_1000_2.5_1

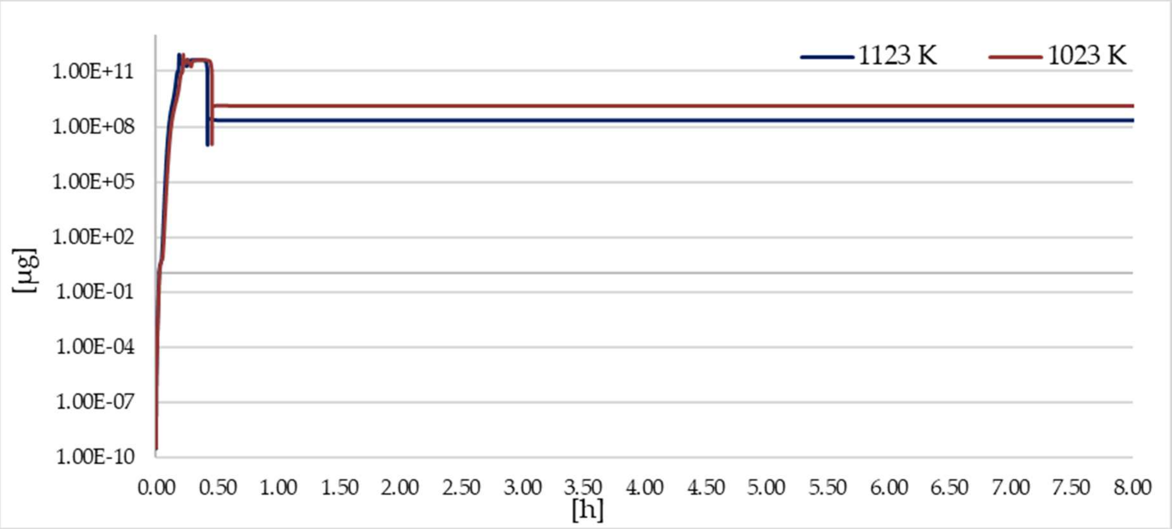


Fig. 39 *Carbon Monoxide*

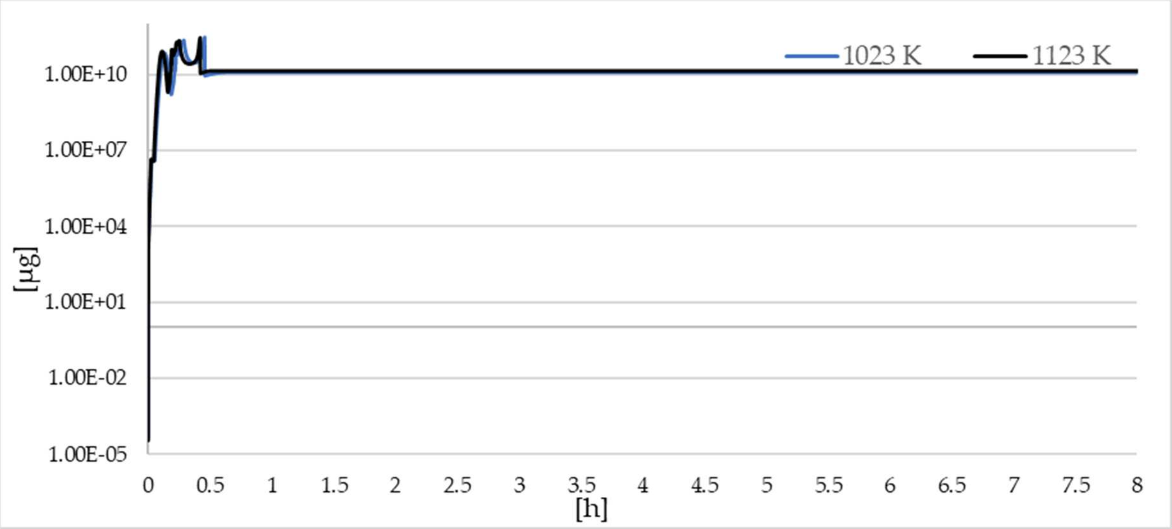


Fig. 40 *Carbon Dioxide*

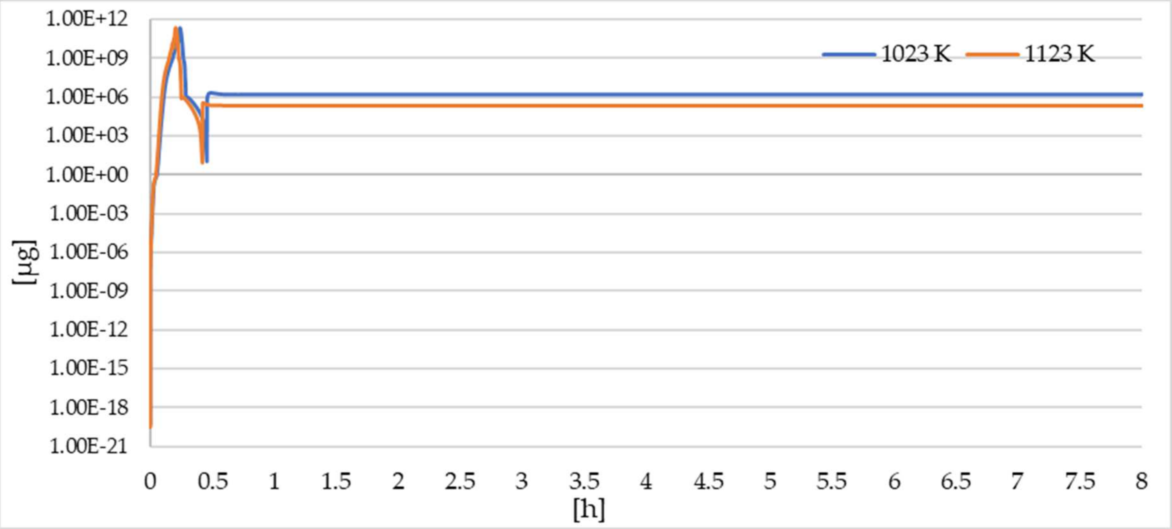


Fig. 41 *Hydrogen*

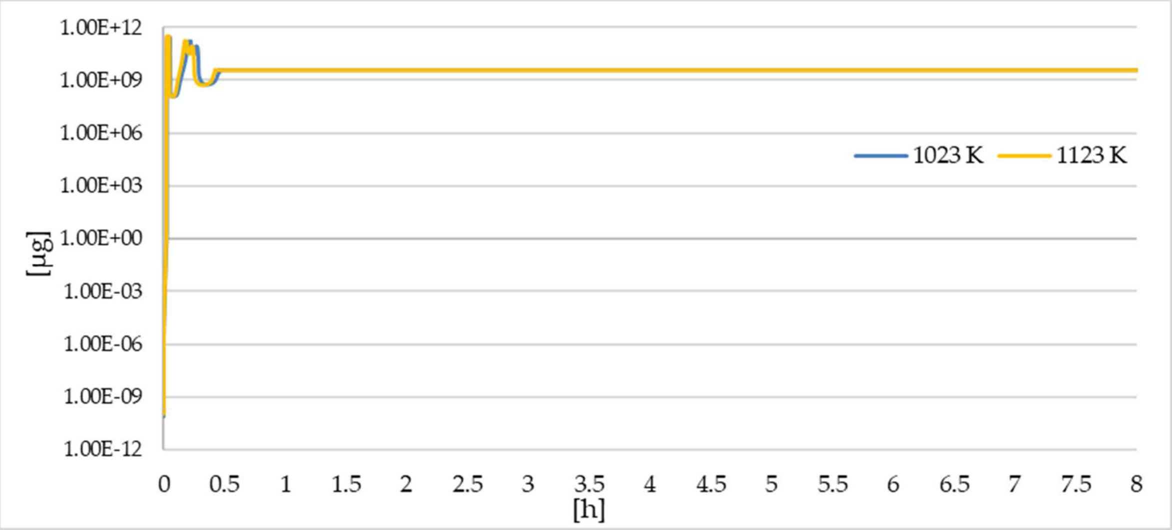


Fig. 42 *Water vapour*

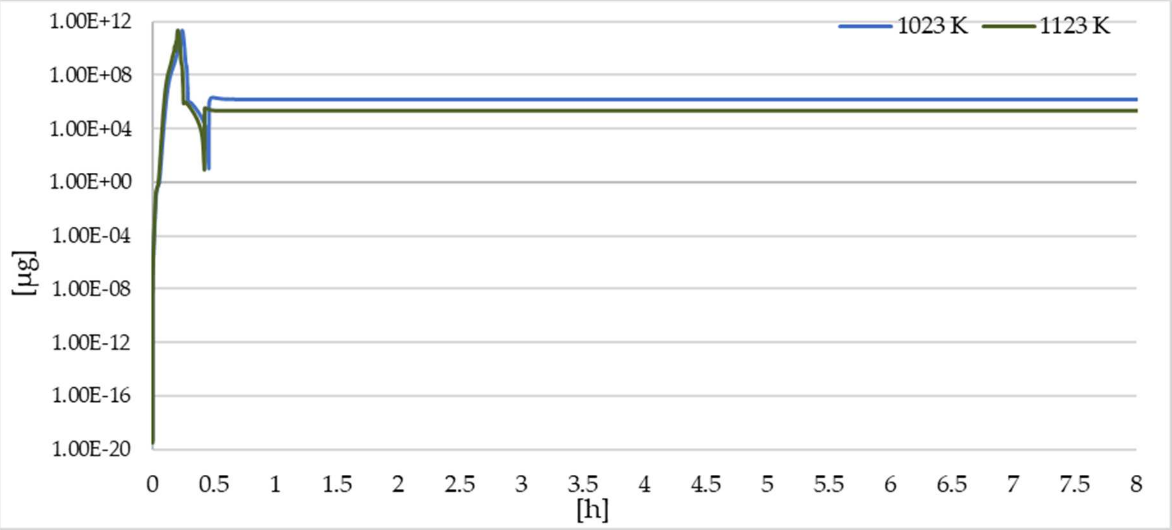


Fig. 43 *Methane*

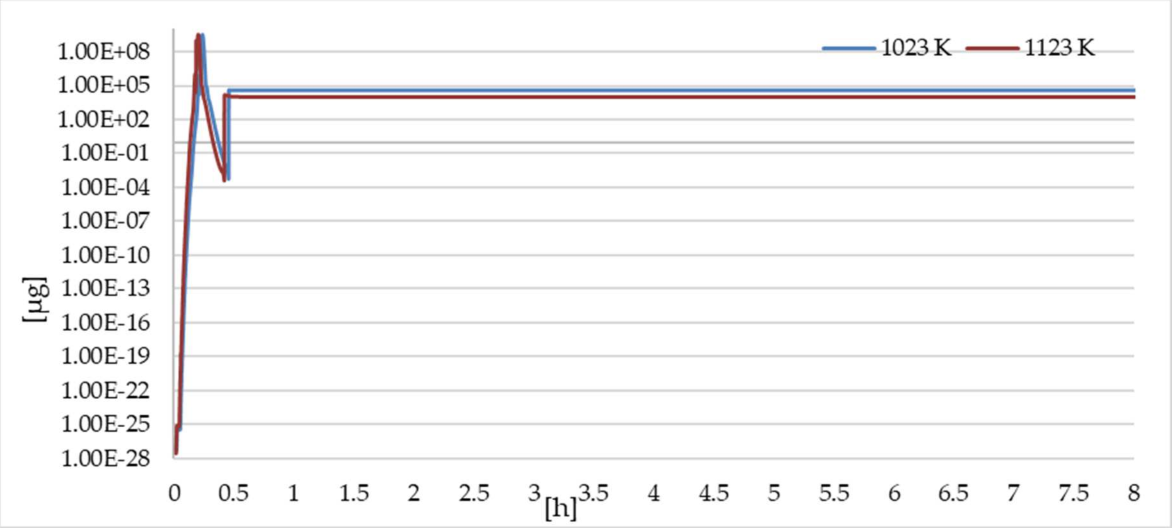


Fig. 44 *Propylene*

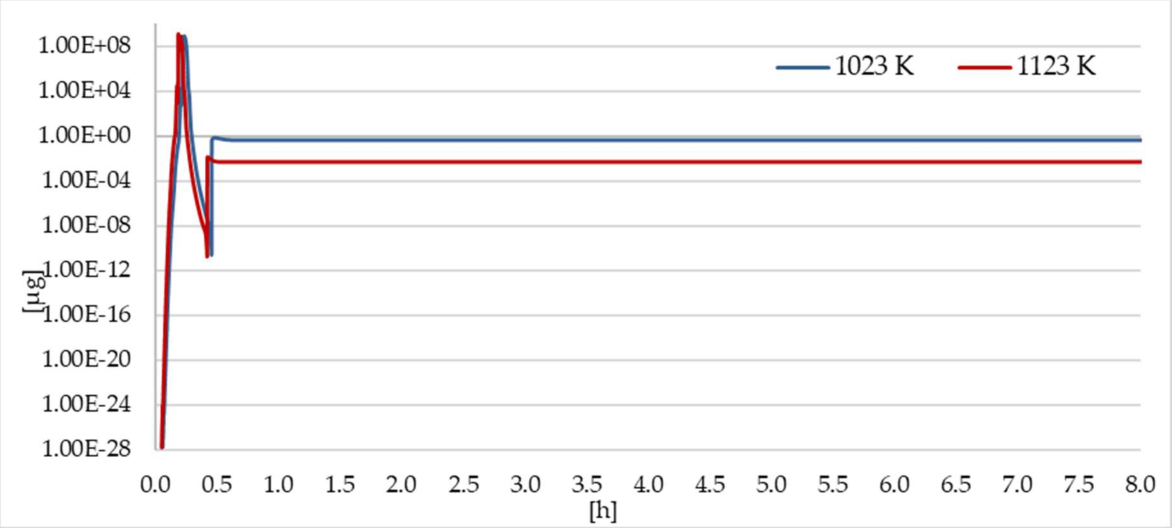


Fig. 45 *Propane*

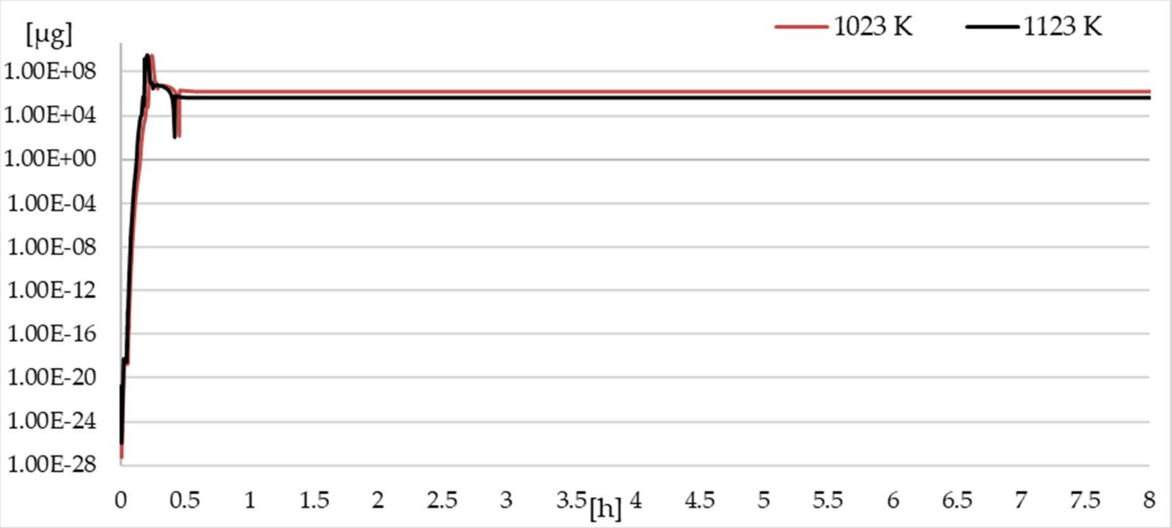


Fig. 46 *Acetylene*

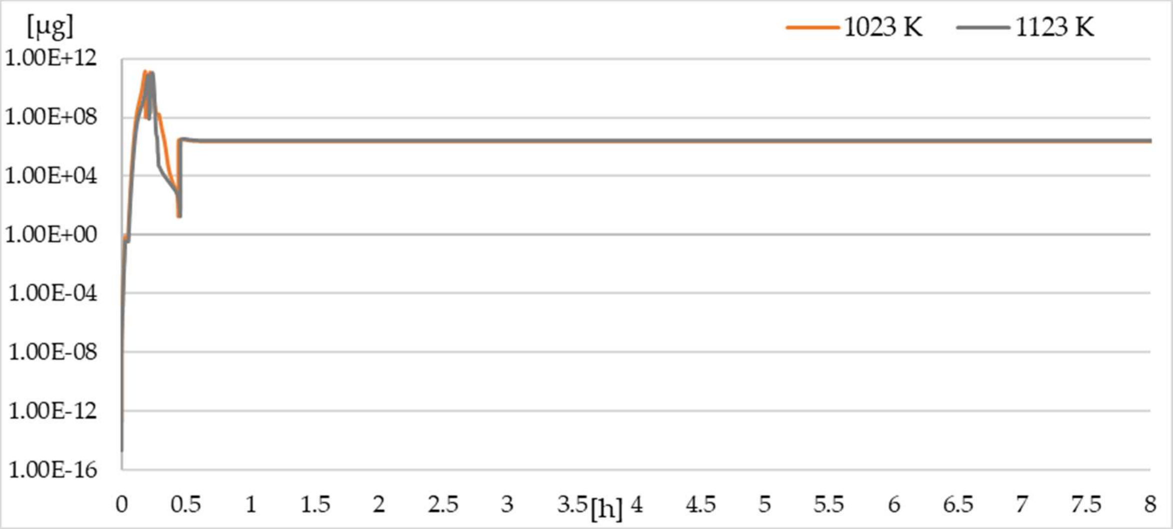


Fig. 47 *Ethylene*

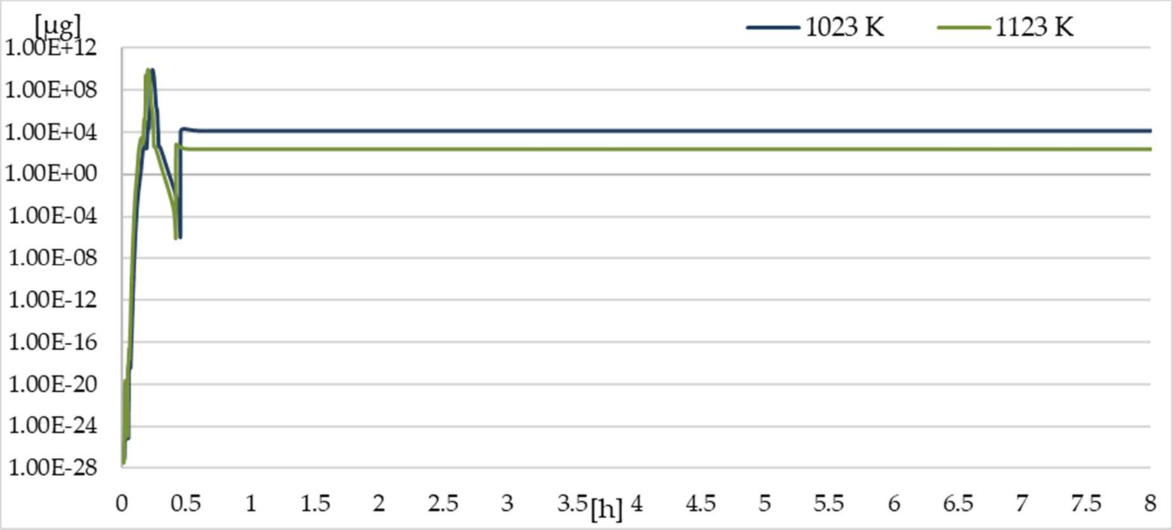


Fig. 48 *Ethene*

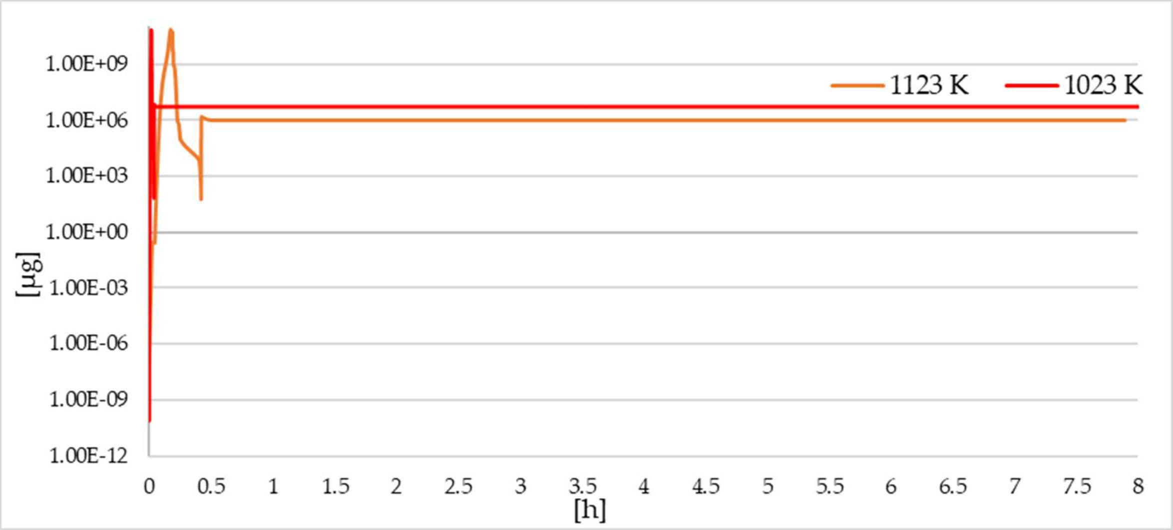


Fig. 49 *Formaldehyde*

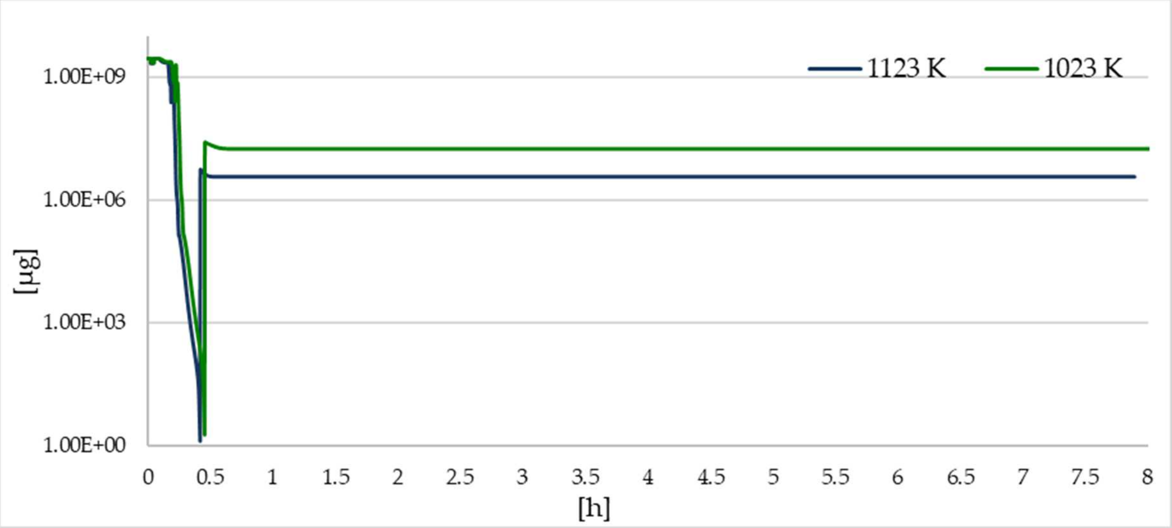


Fig. 50 *Toluene*

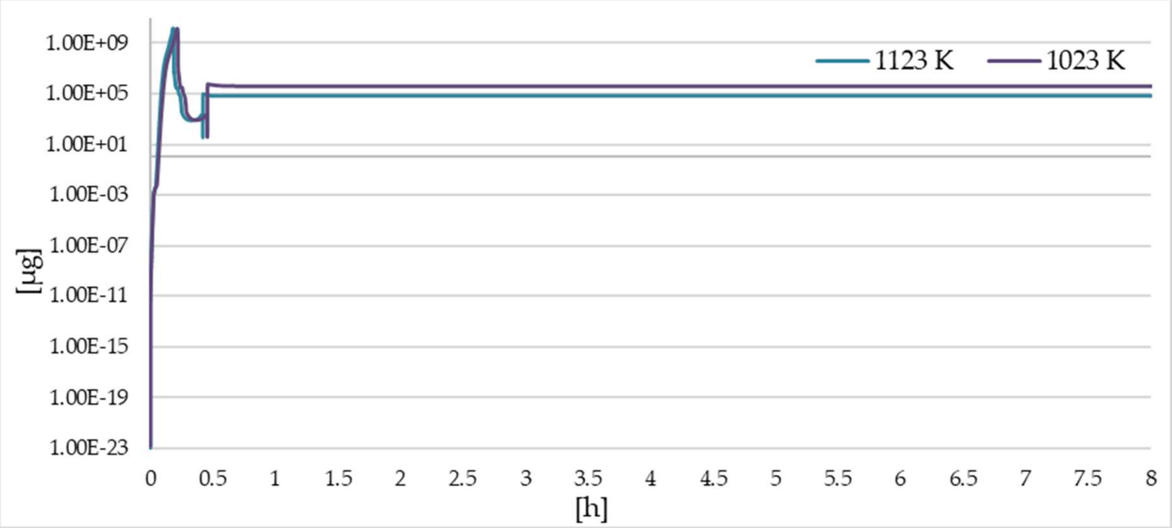


Fig. 51 *Formic Acid*

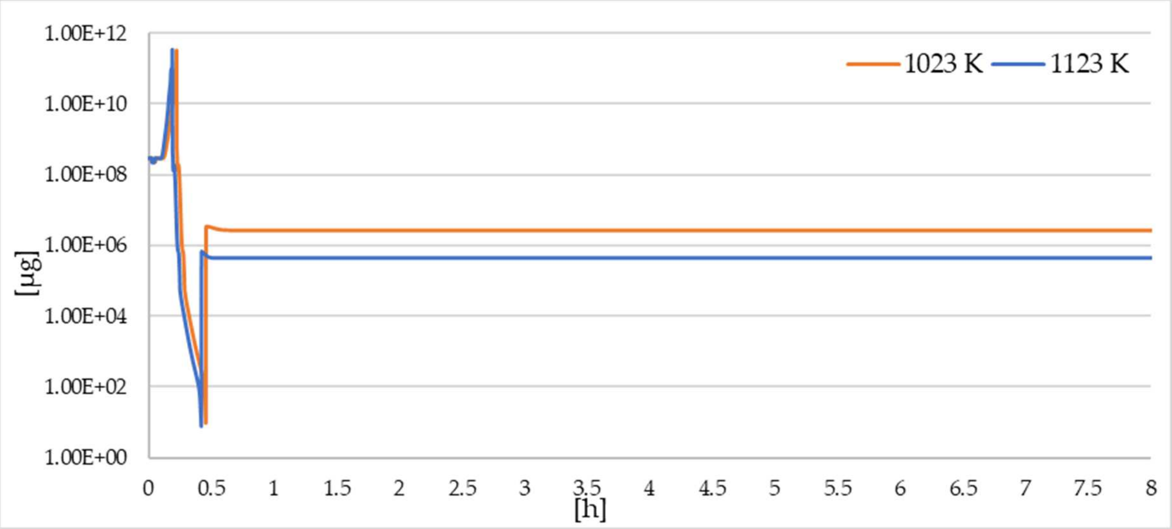


Fig. 52 *Methanol*

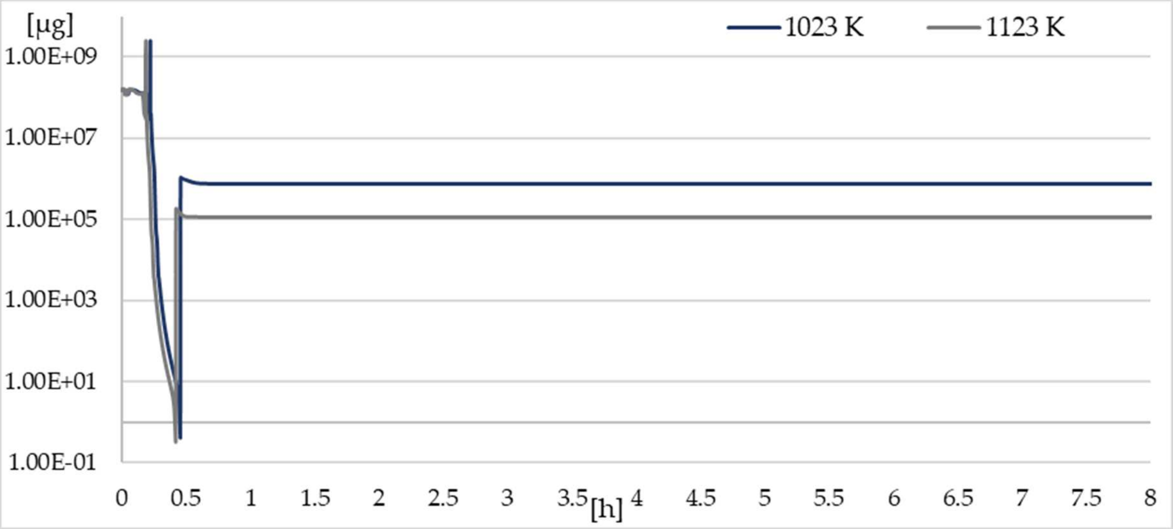


Fig. 53 *Ethanol*

From the previous graphs, it clearly appears that there is a fluctuation in the amount of substances during the start-up phase. The phenomenon is probably due to the ignition of combustion, the biomass pyrolysis, and the generation of reaction intermediates. Within the first hour, the system becomes fully operative, and the output value of the various compounds is steady.

Regarding the temperature of the reactor and biomass, as expected, there is a rapid increase until the maximum is reached within the first hour of operation (Fig. 54 and 55). As for the previously mentioned compounds.

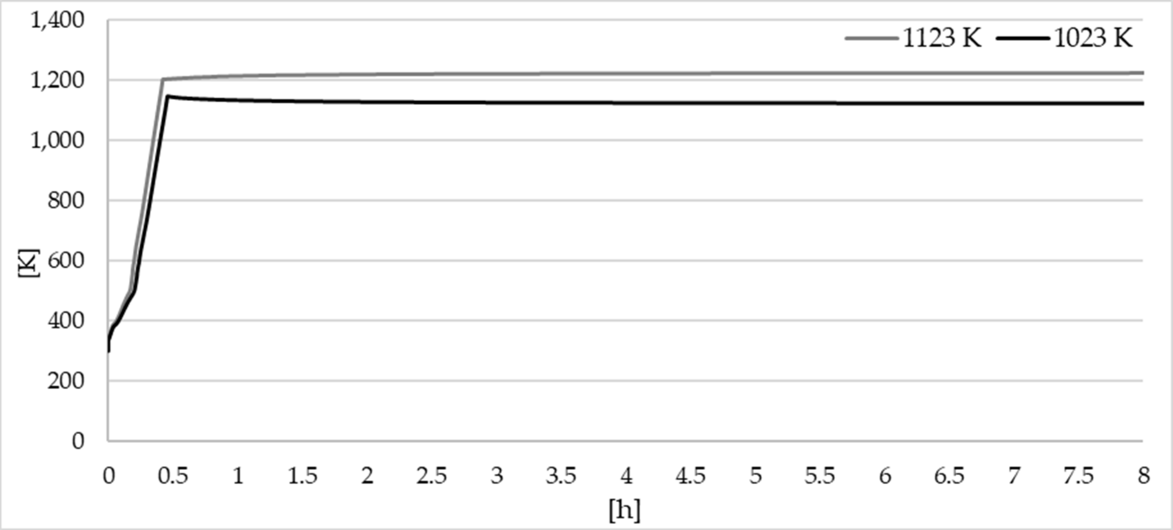


Fig. 54 *Reactor volume temperature*

The reactor was assumed to be adiabatic, so the final temperature is higher as there is no exchange with the environment.

The evaluation of the recoverable heat will be presented in paragraph 9.2.

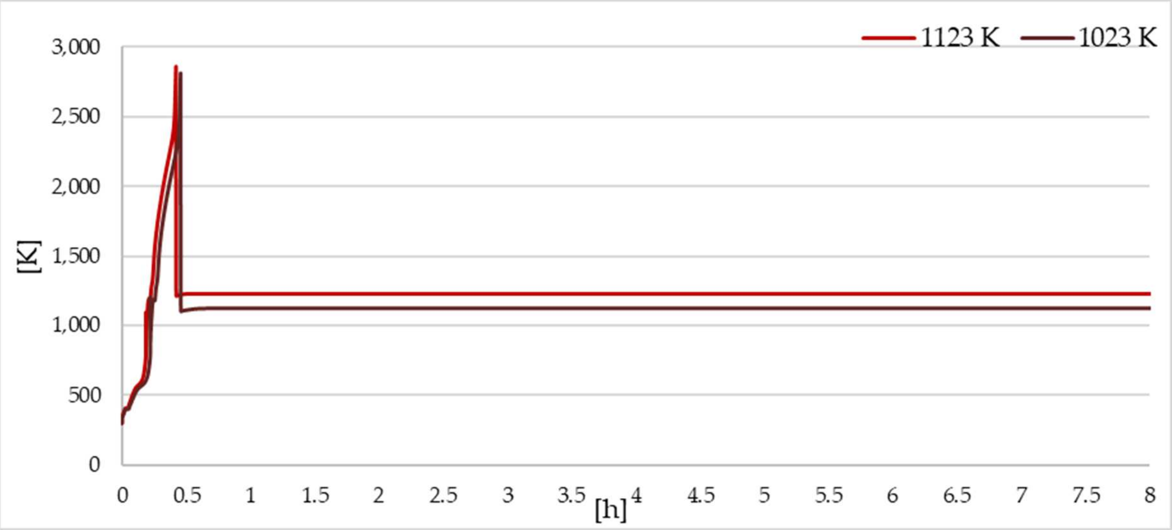


Fig. 55 *Biomass Temperature*

SW_VOC_1000_2.5_1

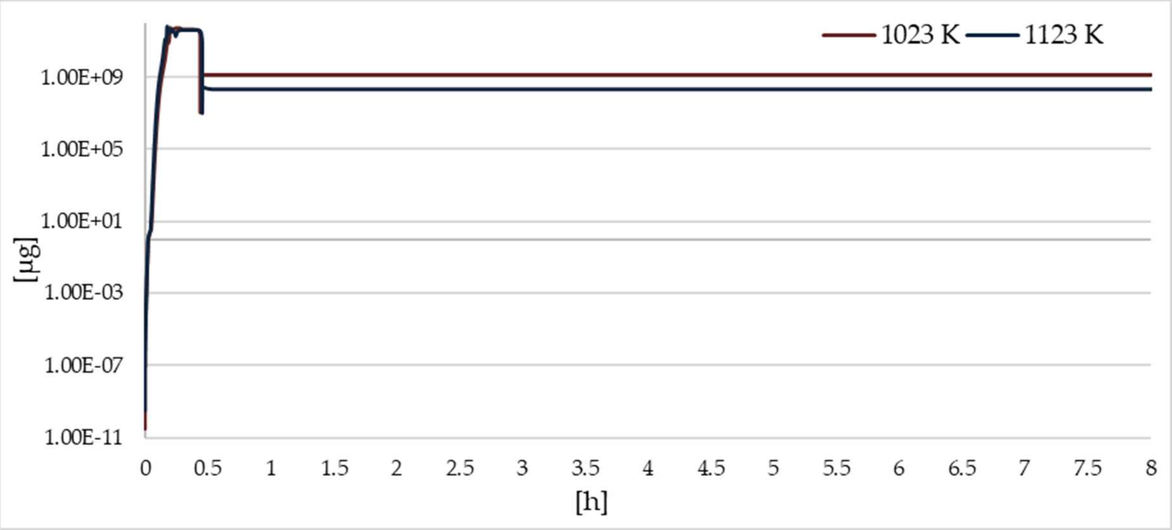


Fig. 56 *Carbon Monoxide*

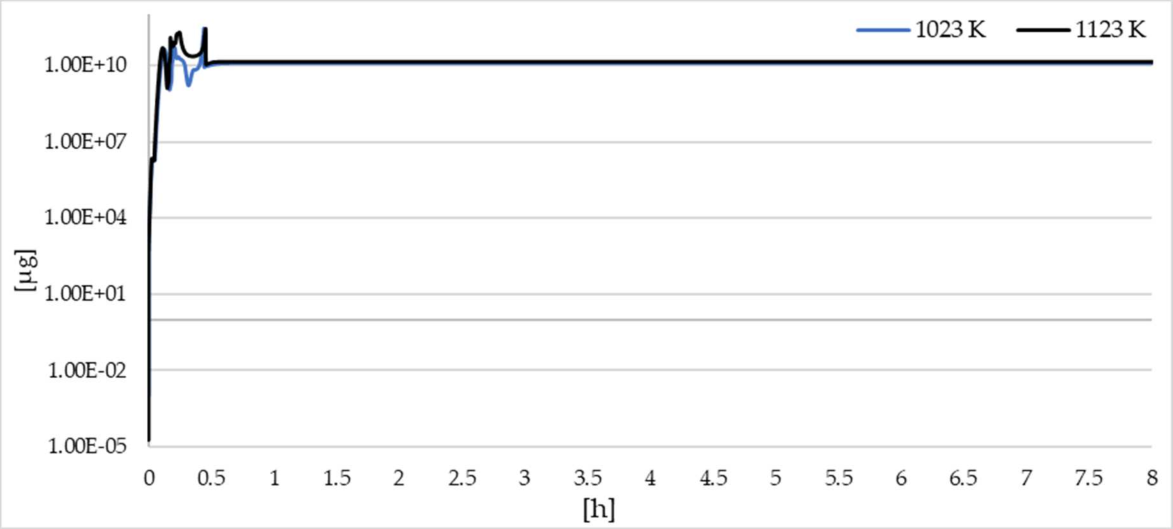


Fig. 57 *Carbon Dioxide*

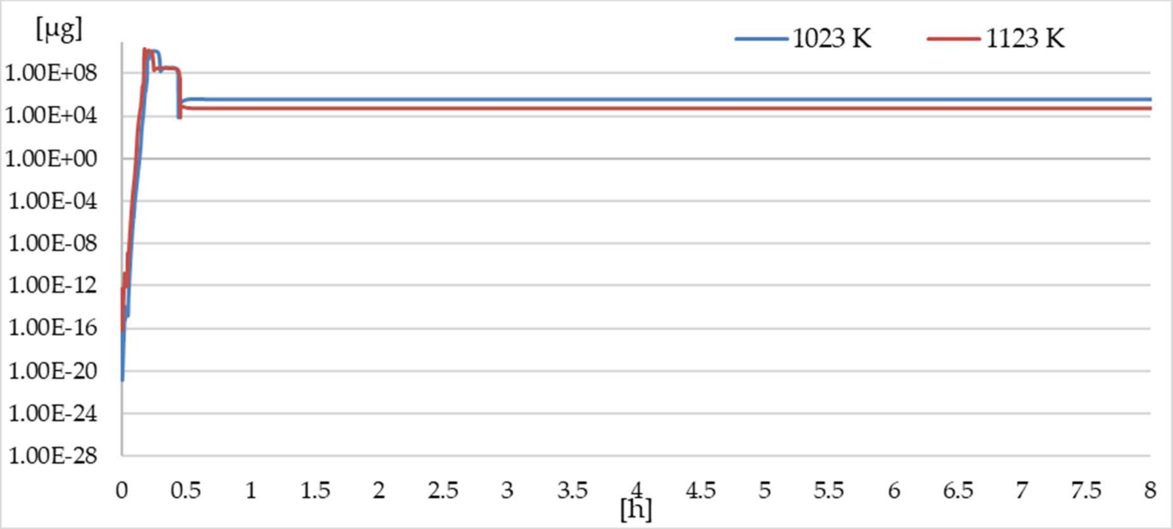


Fig. 58 *Hydrogen*

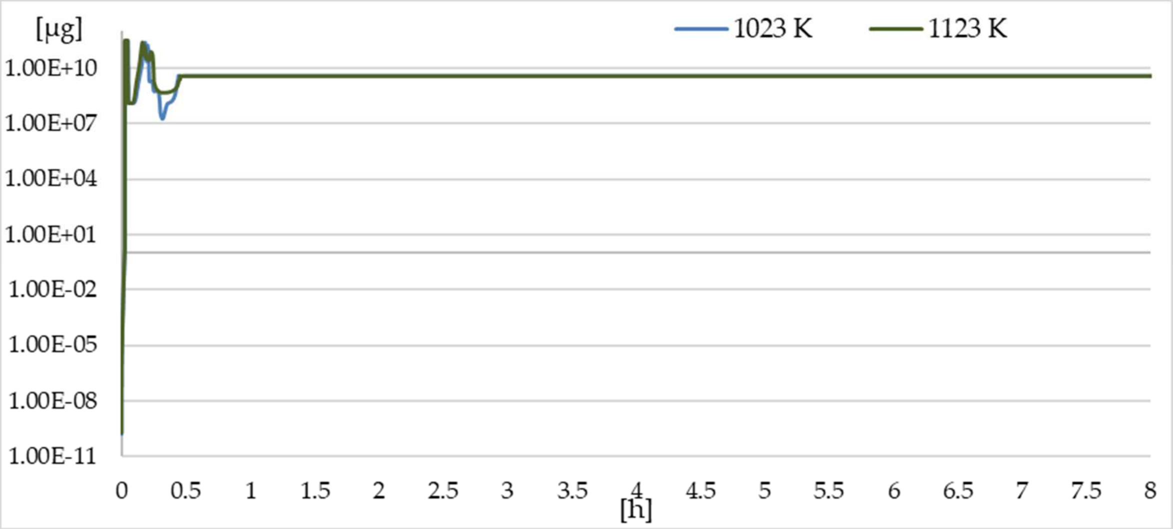


Fig. 59 *Water vapour*

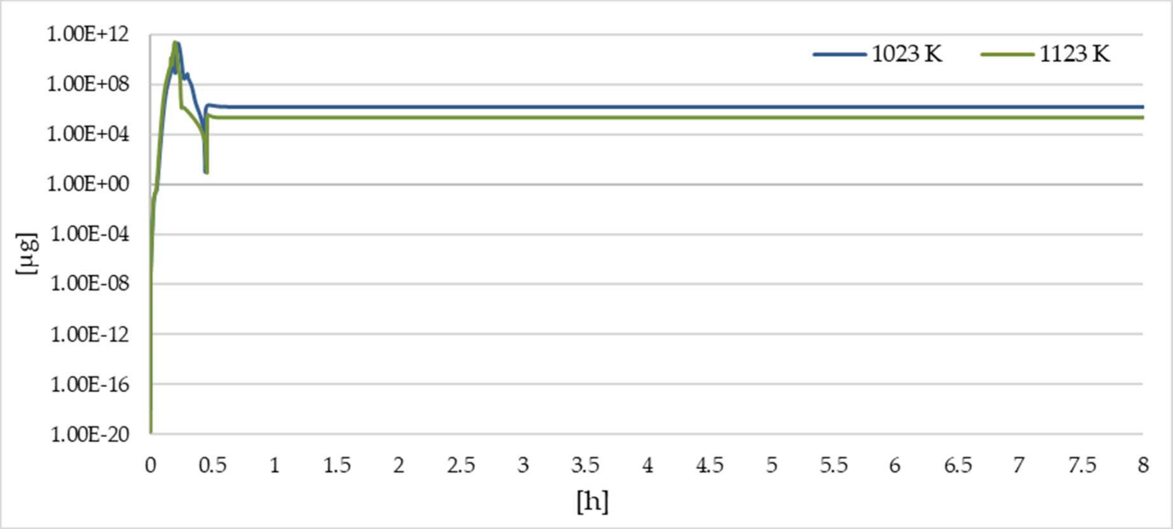


Fig. 60 *Methane*

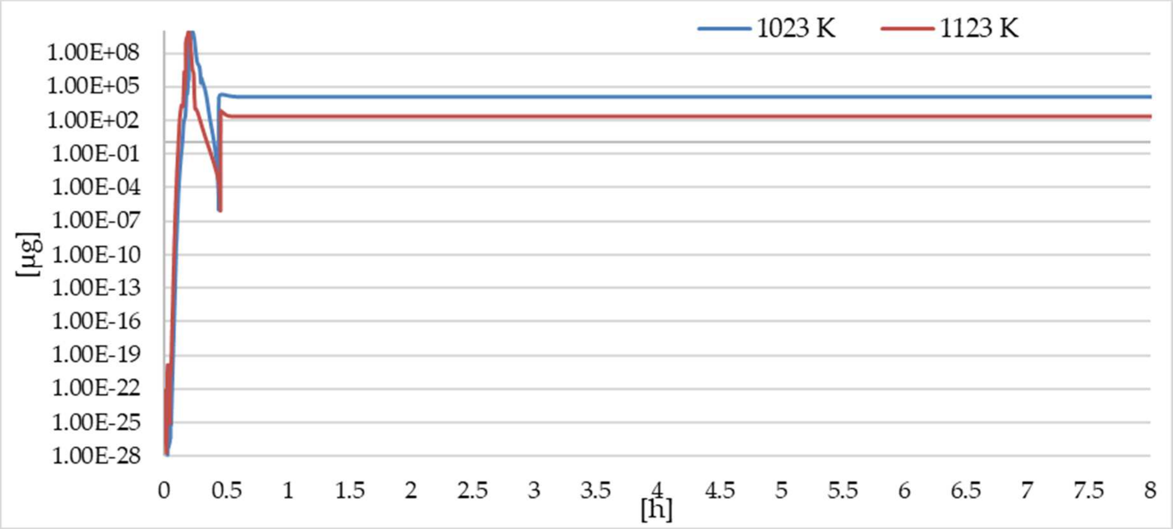


Fig. 61 *Ethane*

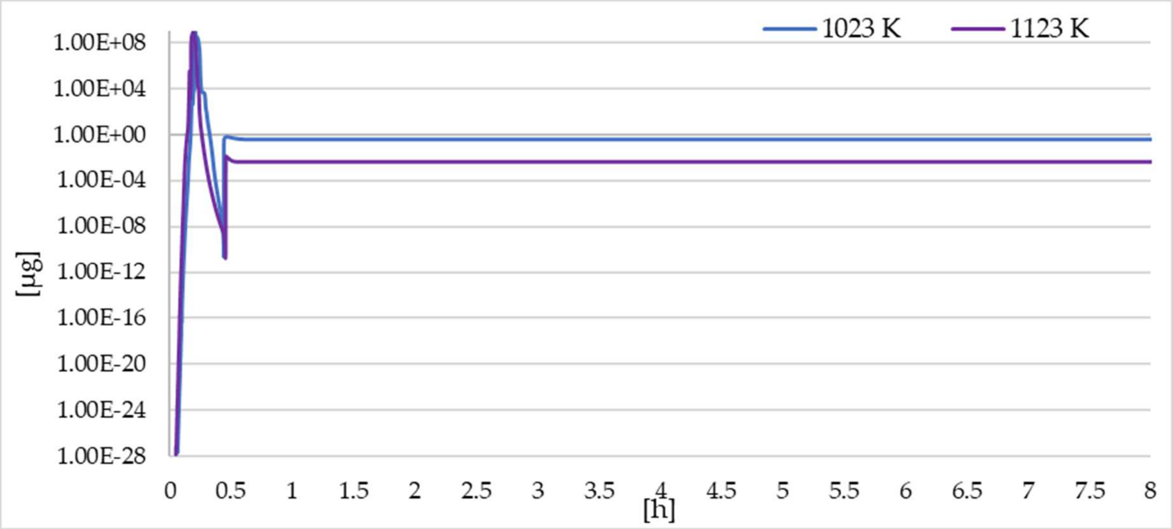


Fig. 62 *Propane*

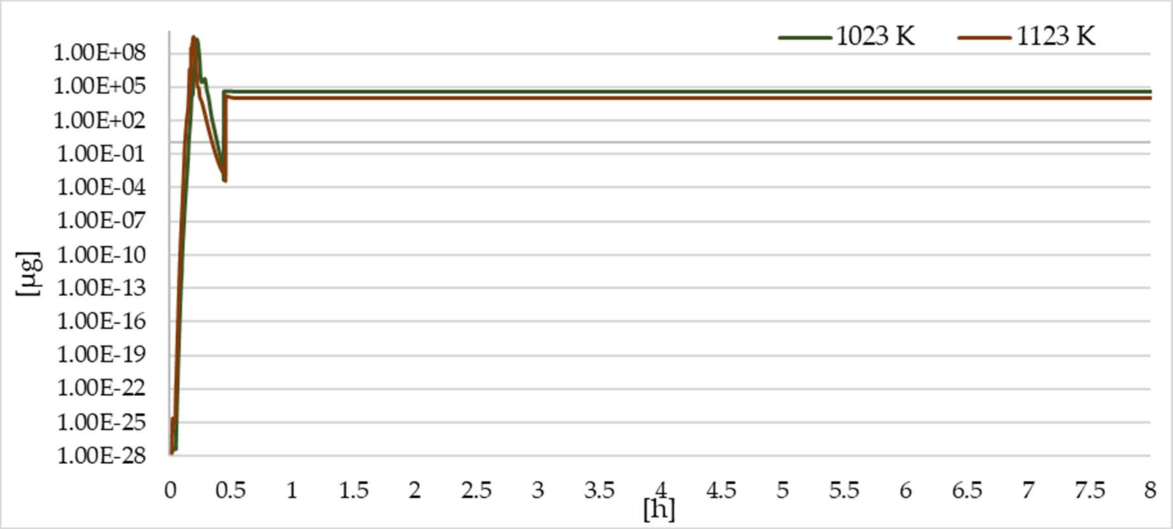


Fig. 63 *Propylene*

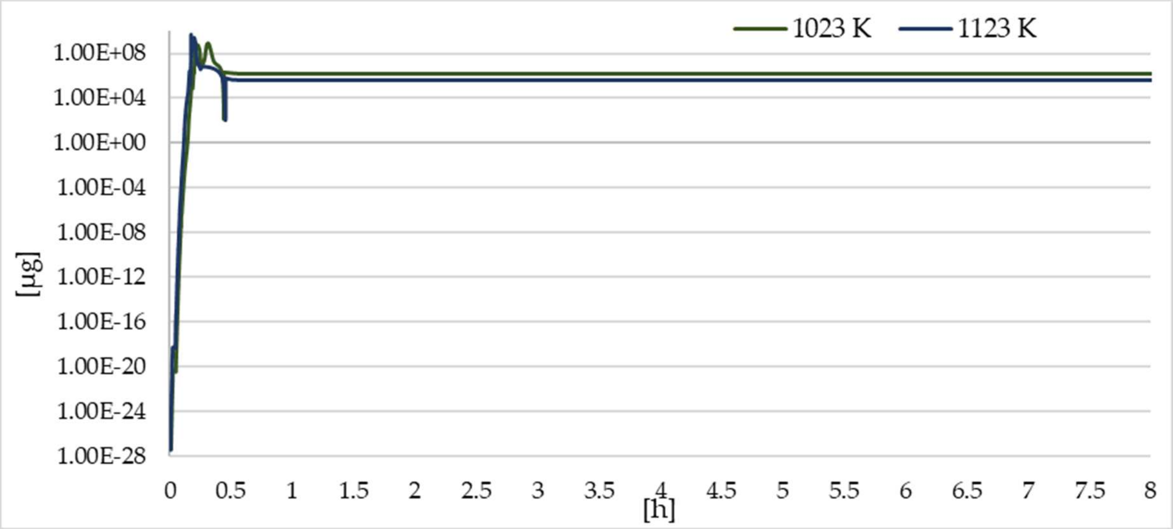


Fig. 64 *Acetylene*

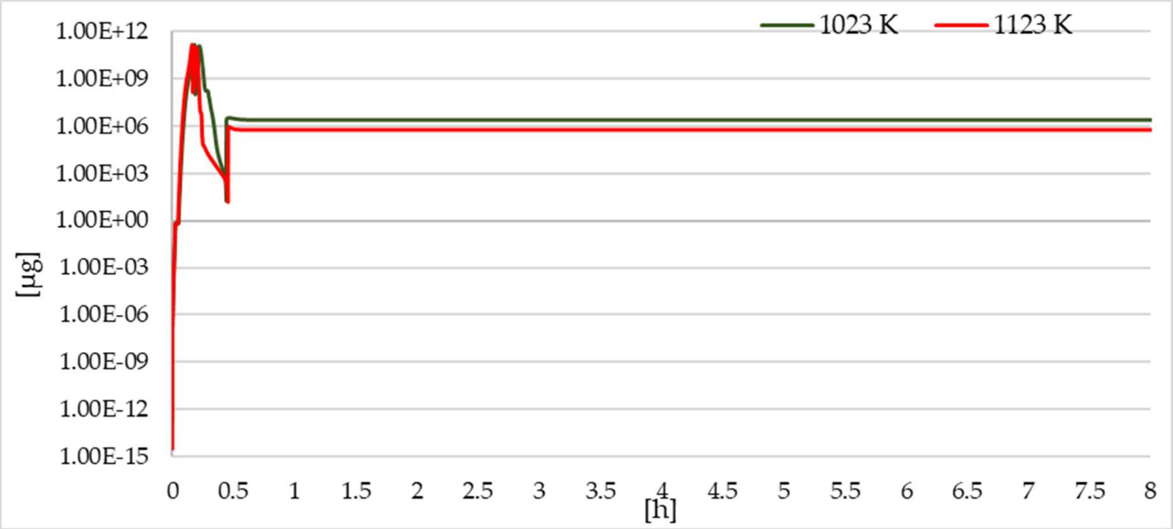


Fig. 65 *Ethylene*

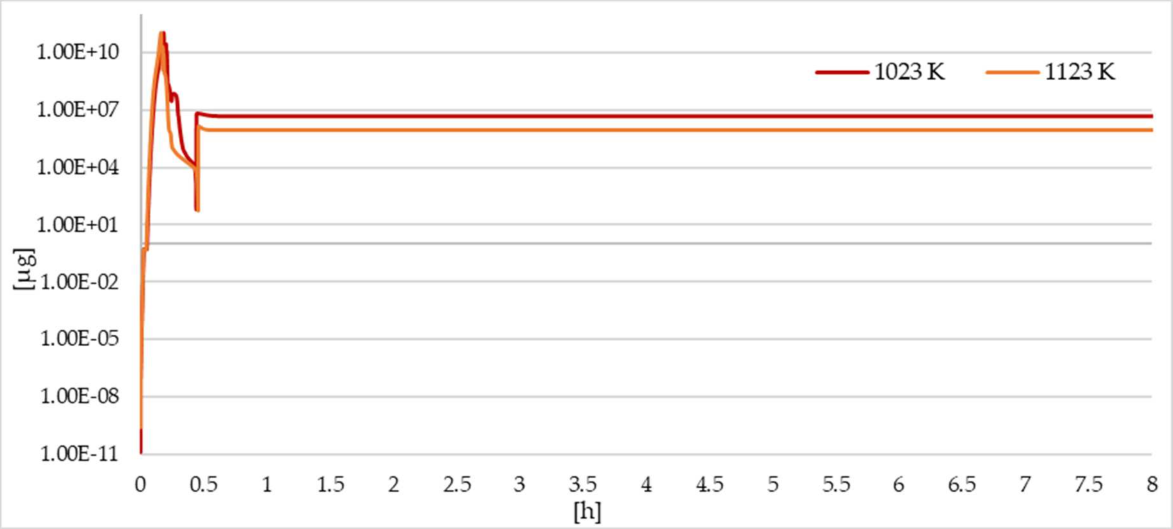


Fig. 66 *Formaldehyde*

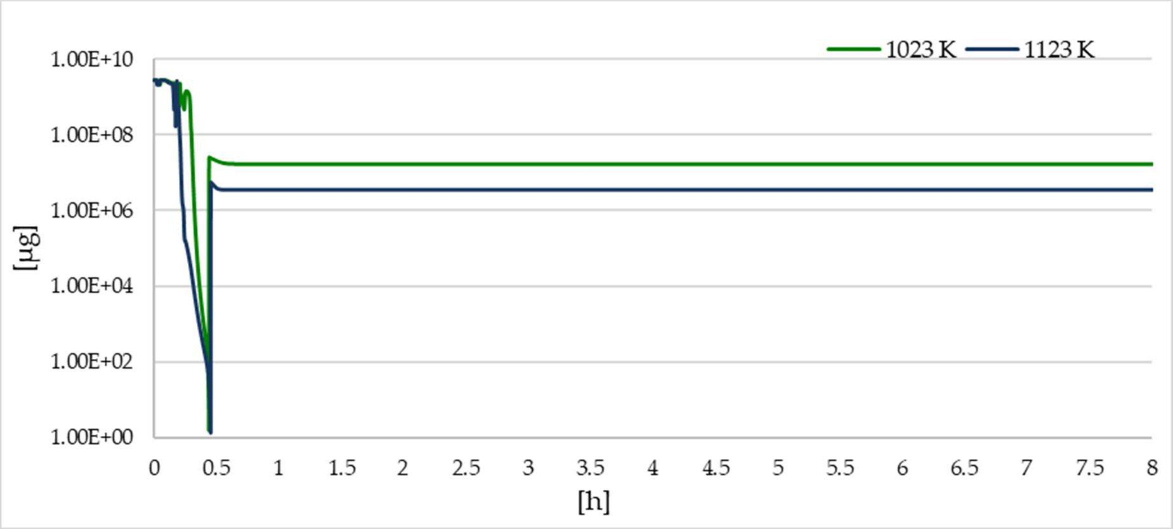


Fig. 67 *Toluene*

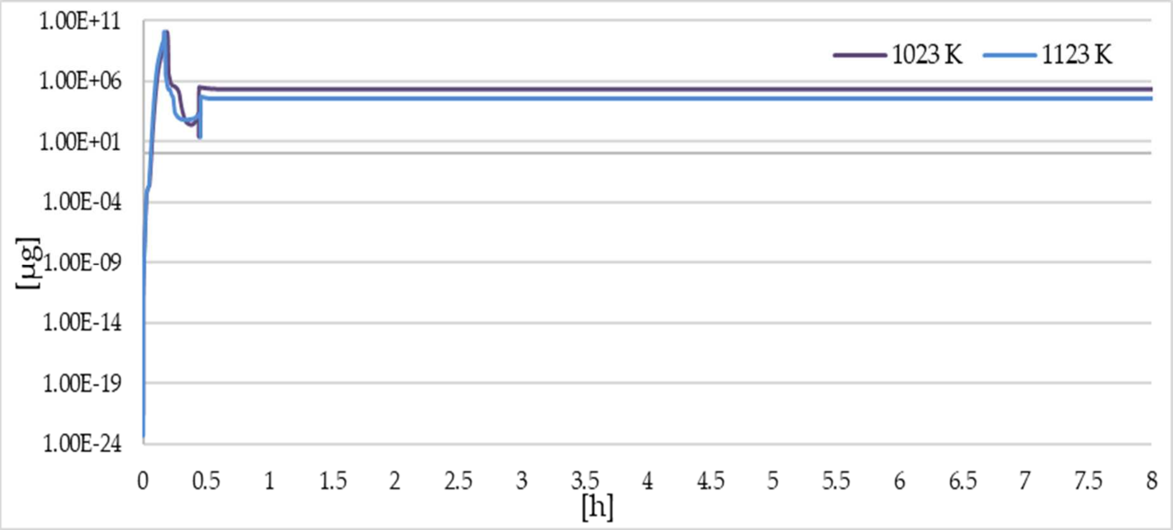


Fig. 68 *Formic Acid*

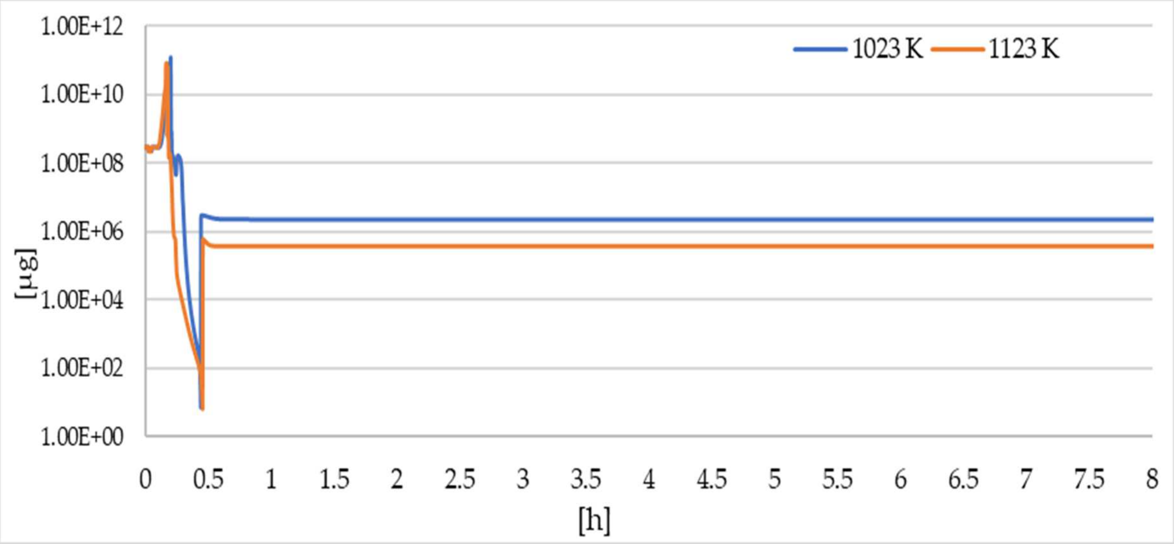


Fig. 69 *Methanol*

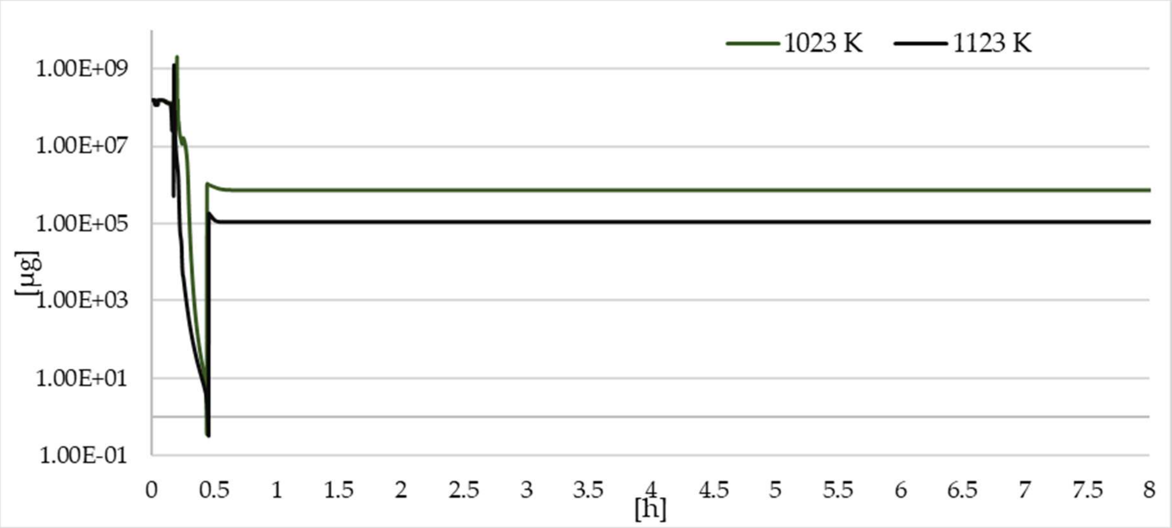


Fig. 70 *Ethanol*

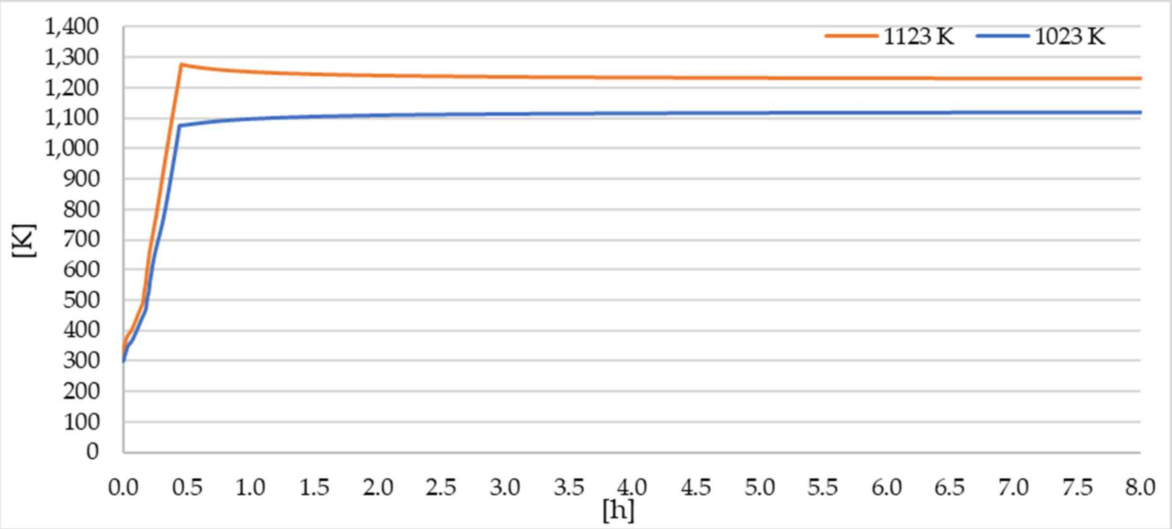


Fig. 71 *Reactor volume temperature*

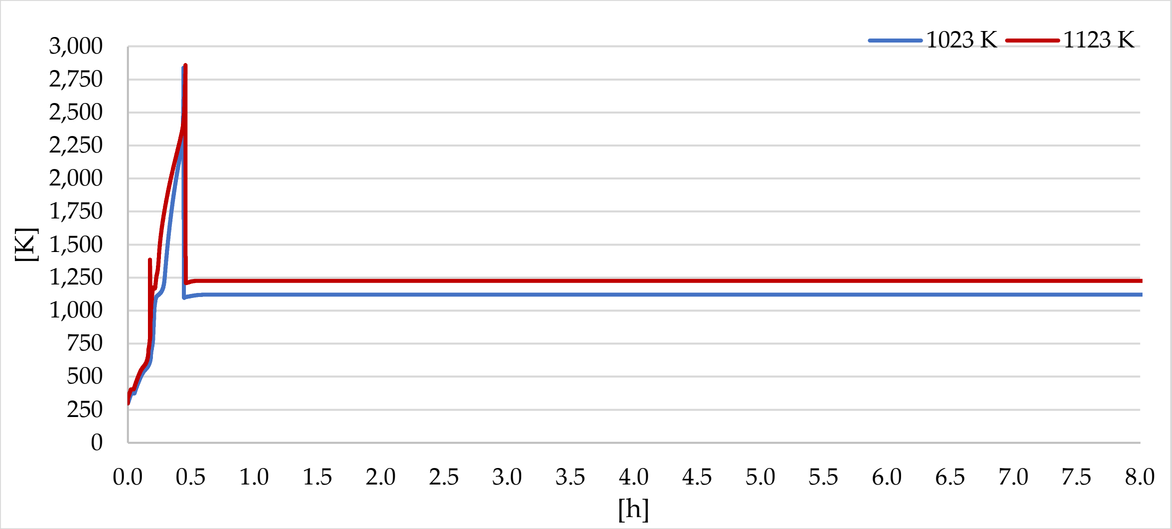


Fig. 72 *Biomass temperature*

9.4. THERMAL ENERGY RECOVERY

This section investigates the potential heat recoverable from the combustion in the reactor volume. As an adiabatic system has been modelled, all the thermal energy generated in the reactor is stored inside. In this thermodynamic configuration there is an increase in the internal temperature. This was evaluated, in average, for the simulations around 100 K, as difference (ΔT) between the starting T_{IN} and the last $T_{Steady\ state}$ (where T_{IN} is the selected temperature to evaluate in the scenario and $T_{Steady\ state}$ is the temperature in the steady state within the 8 hour). The values are shown in the following table for Hardwood (Tab. 18), but the same argumentations are valid for the Softwood.

SOFTWOOD	T_{IN} [K]	T_{FIN} [K]	ΔT
SW_VOC_1000_2.5_1_1023	1023	1121.78	98.78
SW_VOC_1000_2.5_1_1043	1043	1143.84	100.84
SW_VOC_1000_2.5_1_1063	1063	1165.29	102.29
SW_VOC_1000_2.5_1_1083	1083	1186.03	103.03
SW_VOC_1000_2.5_1_1103	1103	1206.08	103.08
SW_VOC_1000_2.5_1_1123	1123	1225.71	102.71
SW_VOC_1000_2.5_4_1023	1023	1129.12	106.12
SW_VOC_1000_2.5_4_1043	1043	1149.4	106.4
SW_VOC_1000_2.5_4_1063	1063	1169.24	106.24

SW_VOC_1000_2.5_4_1083	1083	1188.68	105.68
SW_VOC_1000_2.5_4_1103	1103	1207.94	104.94
SW_VOC_1000_2.5_4_1123	1123	1227.33	104.33
SW_VOC_1000_10_1_1023	1023	1222.66	199.66
SW_VOC_1000_10_1_1043	1043	1241.87	198.87
SW_VOC_1000_10_1_1063	1063	1261.13	198.13
SW_VOC_1000_10_1_1083	1083	1280.53	197.53
SW_VOC_1000_10_1_1103	1103	1300.05	197.05
SW_VOC_1000_10_1_1123	1123	1319.66	196.66
SW_VOC_1000_10_4_1023	1023	1224.96	201.96
SW_VOC_1000_10_4_1043	1043	1243.99	200.99
SW_VOC_1000_10_4_1063	1063	1263.31	200.31
SW_VOC_1000_10_4_1083	1083	1282.83	199.83
SW_VOC_1000_10_4_1103	1103	1302.47	199.47
SW_VOC_1000_10_4_1123	1123	1322.2	199.2
SW_VOC_5000_2.5_1_1023	1023	1079.91	56.91
SW_VOC_5000_2.5_1_1043	1043	1103.65	60.65
SW_VOC_5000_2.5_1_1063	1063	1127.09	64.09
SW_VOC_5000_2.5_1_1083	1083	1150.27	67.27
SW_VOC_5000_2.5_1_1103	1103	1173.16	70.16
SW_VOC_5000_2.5_1_1123	1123	1195.62	72.62
SW_VOC_5000_2.5_4_1023	1023	1095.22	72.22
SW_VOC_5000_2.5_4_1043	1043	1117.22	74.22
SW_VOC_5000_2.5_4_1063	1063	1138.86	75.86
SW_VOC_5000_2.5_4_1083	1083	1160.06	77.06
SW_VOC_5000_2.5_4_1103	1103	1180.74	77.74
SW_VOC_5000_2.5_4_1123	1123	1200.88	77.88
SW_VOC_5000_10_1_1023	1023	1097.35	74.35
SW_VOC_5000_10_1_1043	1043	1122.01	79.01
SW_VOC_5000_10_1_1063	1063	1146.26	83.26
SW_VOC_5000_10_1_1083	1083	1170.1	87.1
SW_VOC_5000_10_1_1103	1103	1193.36	90.36
SW_VOC_5000_10_1_1123	1123	1215.64	92.64
SW_VOC_5000_10_4_1023	1023	1115.14	92.14
SW_VOC_5000_10_4_1043	1043	1137.21	94.21
SW_VOC_5000_10_4_1063	1063	1158.73	95.73
SW_VOC_5000_10_4_1083	1083	1179.61	96.61
SW_VOC_5000_10_4_1103	1103	1199.82	96.82
SW_VOC_5000_10_4_1123	1123	1219.54	96.54

Tab. 18 *Reactor Temperature in the Hardwood simulations*

Therefore, it was assumed that the heat can be recovered and become available to a heat transfer fluid (such as water, air). To validate the hypothesis, the recoverable thermal energy has been calculated using the following equation (2).

$$Q = m \cdot Cp \cdot \Delta T \tag{2}$$

Where:

- m is the mass flow [kg/s] of every compound;
- Cp [kJ/kg/K] is the specific heat for every compound involved (air, VOCs, and biomass);
- ΔT [K] = $T_0 - T_{fin}$ in the reactor.

The total Cp for VOCs was calculated as the weighted average of the Cp of each VOC (from literature) divide by the whole mass. The following tables resume the values used to obtain the recoverable thermal energy for softwood and hardwood combustion.

	Cp,gas at T= 298.15 K [J/mol*K]	**MASS FLOW*** [kg/s]
Acetone	75.02	0.00015
Toluene	158.7	0.000094
MEK	101.68	0.000031
Xylen	126	0.000039
Ethanol	65.21	0.000041
AIR	1004.5	0.33333

* Referred to Total Flow = 1000 Nm^3/h

Tab. 19 *Base data for air and VOCs*

	Specific enthalpy * **h** [kcal/kg]	**Specific enthalpy h [J/kg]**
Hardwood	5380.18	22525738
Softwood	5635.49	23594670

* As an output from GasDs

Tab. 20 *Specific enthalpy of the two types of biomasses*

Biomass feed	**Recoverable thermal energy**	
[kg/h]	Softwood	Hardwood
2.5	49917 J/s	49175 J/s
10	99073 J/s	96103 J/s

Tab. 21 *Recoverable thermal energy by softwood and hardwood biomass burning.*

10.CONCLUSION

This research work focused on the preliminary study of an alternative system combining the combustion of virgin waste wood and the thermal destruction of VOCs from the wood coating processes.

Different scenarios were analysed by simulating the consumption of softwood and hardwood biomass. In addition, were considered different regime temperatures for the operation of the combustion chamber. The software used was GasDs, which modelled a perfectly mixed and adiabatic continuous reactor into where representative VOCs were fed. The concentration of these pollutants was obtained from the mass balance of solvents used by a company taken as a case study. In addition, a different amount of biomass to be burnt was also considered to observe the thermal and abatement performance.

The flexibility of the GasDs kinetic model, which can be easily adapted and modified, is a key aspect of this tool and allows the model to be refined based on new experimental information.

The first result to be highlighted is that the simulations showed the compatibility between biomass combustion and the thermal abatement of certain pollutants in an air stream. This 'compatibility' responds to the first and most important question posed in this PhD research.

The second result, that can be observed from the simulations, is a high VOC abatement. This is evident from output concentrations in the order of μg/h instead of traditionally mg/h. Of course, these abatement efficiencies rise as the operating temperature in the combustion volume increases.

Moreover, the output concentration profiles as a function of operating time, of the main solvents investigated, illustrate that the phenomenon comes into steady state within the first hour from the start-up.

10.1. POSSIBLE CRITICISMS AND THEIR MITIGATIONS

- Regarding the gases naturally emitted at the output of biomass combustion, such as SOx and NOx, were not analysed in this study. However, their formation and concentration can be easily managed with monitoring and abatement systems. In the case of NOx with the well-known urea injection system.
- About the dust content of the emission, it can be divided into inorganic residue and the fraction of carbonaceous particles, soot or organic agglomerates related to the quality of combustion. Depending on the type of fuel and combustion mode, these residues are distributed between bottom ash, which is collected under the furnace, and fly ash, which is transported with the combustion gases. These PMs can be managed by installing downstream abatement systems such as cyclones, electrostatic precipitators, or bag filters.
- The recoverable thermal power was calculated from both literature data and the output values of the GasDs. Furthermore, according to basic hypothesis on the adiabatic, continuous, and perfectly mixed reactor volume. Consequently, the values obtained must be regarded as an estimation.

The implementation of this unified system aimed to recover energy from waste and to reduce pollutants could offer potential benefits both from an energy-environmental and economic point of view.

10.2. IMPLICATIONS OF THE FINDINGS FOR THE FUTURE RESEARCH

The results obtained from this research are preliminary and are based on certain computational assumptions, such as the continuous and adiabatic reactor chamber. Future investigations will focus on retrofitting some parameters of the equations that regulate the phenomenon and the development of a laboratory-scale system.

Engineering will also be the subject of future research, particularly the use of recoverable thermal power for domestic hot water production or workplace heating.

An additional question that would also need to be investigated is the compatibility with legislation. Currently, the regulations do not allow the simultaneous combustion of virgin biomass and VOCs, because they are conventionally performed by two separate systems (usually Thermal Oxidizers and Biomass boilers).

Future implementations, therefore, will be connected to other discipline-specific competences and validated by experimental evidence.

APPENDIX

This appendix presents the most important tables derived from the output data, achieved in the others GasDs simulations.

Only the tables with the found results have been shown. Nevertheless, if the results were graphed, would be observed a trend in line with those shown above.

HARDWOOD

Mass flow output

HW_VOC_1000_2.5_1 MASS FLOW OUT

T [K]	1023	1043	1063	1083	1103	1123
	[µg/Nm^3]	[µg/Nm^3]	[µg/Nm^3]	[µg/Nm^3]	[µg/Nm^3]	[µg/Nm^3]
H2	3.58E+05	2.56E+05	1.77E+05	1.19E+05	7.80E+04	5.21E+04
H2O	3.78E+09	3.79E+09	3.78E+09	3.77E+09	3.75E+09	3.72E+09
CO	1.35E+09	1.03E+09	7.42E+08	5.06E+08	3.32E+08	2.20E+08
CO2	1.21E+10	1.26E+10	1.30E+10	1.34E+10	1.35E+10	1.36E+10
CH4	1.56E+06	1.10E+06	7.59E+05	5.08E+05	3.34E+05	2.23E+05
C3H6	3.80E+04	3.40E+04	2.88E+04	2.24E+04	1.57E+04	1.03E+04
C3H8	4.27E-01	2.08E-01	9.37E-02	3.80E-02	1.38E-02	4.87E-03
C2H2	1.51E+06	1.19E+06	9.35E+05	7.28E+05	5.61E+05	4.31E+05
C2H4	2.66E+06	2.06E+06	1.57E+06	1.18E+06	8.72E+05	6.38E+05
C2H6	1.29E+04	6.94E+03	3.41E+03	1.52E+03	6.17E+02	2.48E+02
CH2O	5.05E+06	3.76E+06	2.75E+06	1.96E+06	1.37E+06	9.66E+05
CH3OH	2.68E+06	1.98E+06	1.41E+06	9.72E+05	6.53E+05	4.42E+05
HCOOH	3.99E+05	2.81E+05	1.96E+05	1.37E+05	9.51E+04	6.68E+04
C7H8	1.76E+07	1.31E+07	9.65E+06	7.04E+06	5.09E+06	3.69E+06
C2H6O	7.55E+05	5.47E+05	3.83E+05	2.59E+05	1.71E+05	1.15E+05

HW_VOC_1000_2.5_4 MASS FLOW OUT

T [K]	1023	1043	1063	1083	1103	1123
	[µg/Nm^3]	[µg/Nm^3]	[µg/Nm^3]	[µg/Nm^3]	[µg/Nm^3]	[µg/Nm^3]
H2	9.63E+04	6.62E+04	4.38E+04	2.82E+04	1.84E+04	0.00E+00
H2O	3.81E+09	3.81E+09	3.80E+09	3.78E+09	3.76E+09	0.00E+00
CO	4.08E+08	2.84E+08	1.89E+08	1.21E+08	7.78E+07	0.00E+00
CO2	1.37E+10	1.39E+10	1.40E+10	1.40E+10	1.39E+10	0.00E+00
CH4	4.45E+05	3.07E+05	2.04E+05	1.31E+05	8.49E+04	0.00E+00
C3H6	9.12E+03	7.35E+03	5.38E+03	3.49E+03	2.12E+03	0.00E+00
C3H8	1.28E-02	5.64E-03	2.24E-03	7.98E-04	2.78E-04	0.00E+00
C2H2	4.12E+05	3.37E+05	2.72E+05	2.14E+05	1.64E+05	0.00E+00
C2H4	9.35E+05	7.36E+05	5.61E+05	4.08E+05	2.87E+05	0.00E+00
C2H6	1.03E+03	5.00E+02	2.23E+02	9.14E+01	3.65E+01	0.00E+00
CH2O	1.61E+06	1.18E+06	8.39E+05	5.75E+05	3.91E+05	0.00E+00

CH3OH	6.84E+05	4.83E+05	3.30E+05	2.20E+05	1.47E+05	0.00E+00
HCOOH	8.39E+04	5.88E+04	4.10E+04	2.85E+04	2.00E+04	0.00E+00
C7H8	5.62E+06	4.19E+06	3.04E+06	2.15E+06	1.50E+06	0.00E+00
C2H6O	2.04E+05	1.42E+05	9.47E+04	6.14E+04	4.02E+04	0.00E+00
HW_VOC_1000_10_1 MASS FLOW OUT						
T [K]	**1023**	**1043**	**1063**	**1083**	**1103**	**1123**
	[µg/Nm^3]	[µg/Nm^3]	[µg/Nm^3]	[µg/Nm^3]	[µg/Nm^3]	[µg/Nm^3]
H2	1.49E+05	9.80E+04	7.11E+04	5.56E+04	4.56E+04	3.87E+04
H2O	7.73E+09	7.71E+09	7.70E+09	7.70E+09	7.70E+09	7.71E+09
CO	3.53E+08	2.32E+08	1.67E+08	1.30E+08	1.06E+08	8.87E+07
CO2	2.90E+10	2.91E+10	2.92E+10	2.92E+10	2.93E+10	2.94E+10
CH4	6.95E+05	4.57E+05	3.27E+05	2.52E+05	2.03E+05	1.68E+05
C3H6	7.92E+03	4.79E+03	3.19E+03	2.31E+03	1.77E+03	1.40E+03
C3H8	1.99E-02	6.17E-03	2.40E-03	1.11E-03	5.78E-04	3.22E-04
C2H2	4.02E+05	2.99E+05	2.34E+05	1.93E+05	1.65E+05	1.45E+05
C2H4	1.37E+06	9.55E+05	7.10E+05	5.57E+05	4.55E+05	3.81E+05
C2H6	6.79E+02	2.43E+02	1.08E+02	5.80E+01	3.49E+01	2.27E+01
CH2O	1.40E+06	9.54E+05	7.02E+05	5.50E+05	4.50E+05	3.78E+05
CH3OH	7.62E+05	5.05E+05	3.63E+05	2.78E+05	2.22E+05	1.82E+05
HCOOH	2.36E+05	1.64E+05	1.21E+05	9.31E+04	7.41E+04	6.01E+04
C7H8	3.10E+06	2.19E+06	1.64E+06	1.30E+06	1.07E+06	8.98E+05
C2H6O	8.94E+04	5.95E+04	4.31E+04	3.34E+04	2.71E+04	2.25E+04
HW_VOC_1000_10_4 MASS FLOW OUT						
T [K]	**1023**	**1043**	**1063**	**1083**	**1103**	**1123**
	[µg/Nm^3]	[µg/Nm^3]	[µg/Nm^3]	[µg/Nm^3]	[µg/Nm^3]	[µg/Nm^3]
H2	3.51E+04	2.52E+04	1.95E+04	1.60E+04	1.35E+04	1.17E+04
H2O	7.75E+09	7.74E+09	7.74E+09	7.75E+09	7.76E+09	7.78E+09
CO	8.35E+07	5.95E+07	4.59E+07	3.73E+07	3.12E+07	2.66E+07
CO2	2.95E+10	2.95E+10	2.96E+10	2.96E+10	2.97E+10	2.97E+10
CH4	1.74E+05	1.23E+05	9.35E+04	7.48E+04	6.18E+04	5.21E+04
C3H6	9.15E+02	6.08E+02	4.45E+02	3.44E+02	2.74E+02	2.20E+02
C3H8	4.18E-04	1.65E-04	7.72E-05	4.04E-05	2.27E-05	1.35E-05
C2H2	1.18E+05	9.10E+04	7.45E+04	6.35E+04	5.55E+04	4.94E+04
C2H4	3.94E+05	2.84E+05	2.19E+05	1.77E+05	1.47E+05	1.24E+05
C2H6	3.93E+01	1.75E+01	9.36E+00	5.62E+00	3.63E+00	2.45E+00
CH2O	3.73E+05	2.69E+05	2.08E+05	1.69E+05	1.41E+05	1.20E+05
CH3OH	1.72E+05	1.23E+05	9.42E+04	7.52E+04	6.17E+04	5.15E+04
HCOOH	5.08E+04	3.72E+04	2.85E+04	2.25E+04	1.80E+04	1.46E+04
C7H8	8.70E+05	6.34E+05	4.93E+05	4.00E+05	3.34E+05	2.83E+05
C2H6O	2.12E+04	1.51E+04	1.16E+04	9.37E+03	7.73E+03	6.47E+03
HW_VOC_5000_2.5_1 MASS FLOW OUT						
T [K]	**1023**	**1043**	**1063**	**1083**	**1103**	**1123**
	[µg/Nm^3]	[µg/Nm^3]	[µg/Nm^3]	[µg/Nm^3]	[µg/Nm^3]	[µg/Nm^3]
H2	2.95E+06	2.25E+06	1.69E+06	1.25E+06	8.90E+05	6.13E+05
H2O	1.26E+10	1.29E+10	1.32E+10	1.33E+10	1.34E+10	1.35E+10
CO	1.40E+10	1.26E+10	1.10E+10	9.28E+09	7.45E+09	5.60E+09
CO2	2.45E+10	2.80E+10	3.14E+10	3.48E+10	3.80E+10	4.10E+10

CH4	1.11E+07	8.09E+06	5.81E+06	4.07E+06	2.77E+06	1.82E+06
C3H6	6.74E+05	6.63E+05	6.40E+05	6.00E+05	5.39E+05	4.53E+05
C3H8	2.76E+01	1.78E+01	1.10E+01	6.42E+00	3.49E+00	1.72E+00
C2H2	4.03E+07	3.15E+07	2.45E+07	1.88E+07	1.43E+07	1.06E+07
C2H4	3.14E+07	2.49E+07	1.96E+07	1.52E+07	1.15E+07	8.56E+06
C2H6	3.94E+05	2.70E+05	1.75E+05	1.05E+05	5.82E+04	2.86E+04
CH2O	9.75E+07	7.47E+07	5.66E+07	4.22E+07	3.07E+07	2.18E+07
CH3OH	4.64E+07	3.69E+07	2.90E+07	2.23E+07	1.65E+07	1.17E+07
HCOOH	2.57E+06	1.92E+06	1.41E+06	1.03E+06	7.34E+05	5.16E+05
C7H8	4.87E+08	3.60E+08	2.65E+08	1.94E+08	1.40E+08	9.93E+07
C2H6O	2.00E+07	1.55E+07	1.18E+07	8.85E+06	6.40E+06	4.44E+06
	HW_VOC_5000_2.5_4 MASS FLOW OUT					
T [K]	**1023**	**1043**	**1063**	**1083**	**1103**	**1123**
	[μg/Nm^3]	[μg/Nm^3]	[μg/Nm^3]	[μg/Nm^3]	[μg/Nm^3]	[μg/Nm^3]
H2	7.71E+05	5.77E+05	4.23E+05	3.02E+05	2.11E+05	1.45E+05
H2O	1.35E+10	1.36E+10	1.36E+10	1.36E+10	1.36E+10	1.35E+10
CO	6.57E+09	5.34E+09	4.18E+09	3.11E+09	2.19E+09	1.48E+09
CO2	3.95E+10	4.18E+10	4.38E+10	4.54E+10	4.66E+10	4.74E+10
CH4	2.90E+06	2.10E+06	1.49E+06	1.03E+06	6.94E+05	4.61E+05
C3H6	2.24E+05	2.08E+05	1.87E+05	1.61E+05	1.30E+05	9.56E+04
C3H8	1.29E+00	7.55E-01	4.23E-01	2.22E-01	1.06E-01	4.55E-02
C2H2	1.01E+07	8.00E+06	6.37E+06	5.05E+06	3.99E+06	3.13E+06
C2H4	9.82E+06	7.90E+06	6.32E+06	5.01E+06	3.91E+06	2.99E+06
C2H6	4.98E+04	3.00E+04	1.71E+04	9.12E+03	4.49E+03	2.05E+03
CH2O	2.87E+07	2.20E+07	1.67E+07	1.24E+07	9.07E+06	6.51E+06
CH3OH	1.31E+07	1.02E+07	7.66E+06	5.60E+06	3.96E+06	2.73E+06
HCOOH	6.07E+05	4.35E+05	3.10E+05	2.19E+05	1.55E+05	1.09E+05
C7H8	1.30E+08	9.84E+07	7.40E+07	5.53E+07	4.08E+07	3.00E+07
C2H6O	5.61E+06	4.27E+06	3.17E+06	2.27E+06	1.58E+06	1.07E+06
	HW_VOC_5000_10_1 MASS FLOW OUT					
T [K]	**1023**	**1043**	**1063**	**1083**	**1103**	**1123**
	[μg/Nm^3]	[μg/Nm^3]	[μg/Nm^3]	[μg/Nm^3]	[μg/Nm^3]	[μg/Nm^3]
H2	6.32E+06	4.68E+06	3.39E+06	2.38E+06	1.59E+06	1.03E+06
H2O	1.67E+10	1.71E+10	1.73E+10	1.74E+10	1.75E+10	1.74E+10
CO	1.67E+10	1.44E+10	1.20E+10	9.46E+09	6.94E+09	4.75E+09
CO2	3.67E+10	4.15E+10	4.61E+10	5.05E+10	5.46E+10	5.78E+10
CH4	2.73E+07	1.94E+07	1.36E+07	9.25E+06	6.07E+06	3.89E+06
C3H6	6.31E+05	6.11E+05	5.76E+05	5.18E+05	4.34E+05	3.30E+05
C3H8	5.58E+01	3.16E+01	1.68E+01	8.13E+00	3.49E+00	1.32E+00
C2H2	3.29E+07	2.50E+07	1.89E+07	1.40E+07	1.03E+07	7.42E+06
C2H4	4.46E+07	3.35E+07	2.50E+07	1.83E+07	1.32E+07	9.29E+06
C2H6	5.93E+05	3.77E+05	2.21E+05	1.17E+05	5.42E+04	2.18E+04
CH2O	9.34E+07	6.91E+07	5.05E+07	3.61E+07	2.51E+07	1.72E+07
CH3OH	5.09E+07	3.94E+07	2.99E+07	2.18E+07	1.52E+07	1.01E+07
HCOOH	8.11E+06	5.87E+06	4.19E+06	2.94E+06	2.03E+06	1.38E+06
C7H8	3.71E+08	2.66E+08	1.90E+08	1.34E+08	9.38E+07	6.53E+07
C2H6O	1.58E+07	1.18E+07	8.68E+06	6.16E+06	4.18E+06	2.73E+06

	HW_VOC_5000_10_4 MASS FLOW OUT					
T [K]	**1023**	**1043**	**1063**	**1083**	**1103**	**1123**
	[µg/Nm^3]	[µg/Nm^3]	[µg/Nm^3]	[µg/Nm^3]	[µg/Nm^3]	[µg/Nm^3]
H2	1.61E+06	1.17E+06	8.21E+05	5.58E+05	3.70E+05	2.46E+05
H2O	1.75E+10	1.76E+10	1.76E+10	1.75E+10	1.74E+10	1.73E+10
CO	6.77E+09	5.23E+09	3.85E+09	2.68E+09	1.78E+09	1.17E+09
CO2	5.51E+10	5.77E+10	5.99E+10	6.15E+10	6.24E+10	6.29E+10
CH4	6.96E+06	4.96E+06	3.45E+06	2.34E+06	1.55E+06	1.03E+06
C3H6	1.96E+05	1.77E+05	1.52E+05	1.22E+05	8.89E+04	5.94E+04
C3H8	1.97E+00	1.00E+00	4.74E-01	2.04E-01	7.87E-02	2.84E-02
C2H2	8.02E+06	6.33E+06	4.99E+06	3.91E+06	3.03E+06	2.34E+06
C2H4	1.27E+07	9.88E+06	7.63E+06	5.81E+06	4.33E+06	3.19E+06
C2H6	6.27E+04	3.47E+04	1.77E+04	8.24E+03	3.50E+03	1.43E+03
CH2O	2.60E+07	1.95E+07	1.44E+07	1.04E+07	7.33E+06	5.16E+06
CH3OH	1.34E+07	1.00E+07	7.24E+06	5.05E+06	3.43E+06	2.32E+06
HCOOH	1.75E+06	1.23E+06	8.68E+05	6.07E+05	4.23E+05	2.97E+05
C7H8	9.58E+07	7.16E+07	5.31E+07	3.90E+07	2.83E+07	2.05E+07
C2H6O	4.13E+06	3.03E+06	2.15E+06	1.48E+06	9.85E+05	6.58E+05

Molar fraction output

	HW_VOC_1000_2.5_1 MOLAR FRACTION OUT [%]					
T [K]	**1023**	**1043**	**1063**	**1083**	**1103**	**1123**
N2	7.87E+01	7.87E+01	7.87E+01	7.87E+01	7.87E+01	7.87E+01
O2	2.01E+01	2.01E+01	2.01E+01	2.01E+01	2.01E+01	2.01E+01
H2	3.97E-04	2.84E-04	1.97E-04	1.32E-04	8.65E-05	5.78E-05
H2O	4.68E-01	4.70E-01	4.70E-01	4.68E-01	4.65E-01	4.62E-01
CO	1.08E-01	8.21E-02	5.92E-02	4.04E-02	2.65E-02	1.75E-02
CO2	6.13E-01	6.41E-01	6.63E-01	6.78E-01	6.87E-01	6.91E-01
CH4	2.17E-04	1.53E-04	1.06E-04	7.08E-05	4.66E-05	3.10E-05
C3H6	2.02E-06	1.80E-06	1.53E-06	1.19E-06	8.35E-07	5.46E-07
C3H8	2.16E-11	1.06E-11	4.75E-12	1.92E-12	7.00E-13	2.47E-13
C2H2	1.30E-04	1.02E-04	8.03E-05	6.25E-05	4.82E-05	3.70E-05
C2H4	2.12E-04	1.64E-04	1.25E-04	9.44E-05	6.95E-05	5.08E-05
C2H6	9.61E-07	5.16E-07	2.54E-07	1.13E-07	4.59E-08	1.84E-08
CH2O	3.76E-04	2.80E-04	2.05E-04	1.46E-04	1.02E-04	7.19E-05
CH3OH	1.87E-04	1.38E-04	9.85E-05	6.78E-05	4.56E-05	3.08E-05
HCOOH	1.94E-05	1.36E-05	9.54E-06	6.65E-06	4.62E-06	3.25E-06
C7H8	4.26E-04	3.17E-04	2.34E-04	1.71E-04	1.23E-04	8.96E-05
C2H6O	3.66E-05	2.65E-05	1.86E-05	1.26E-05	8.32E-06	5.57E-06
Σ	99.99	99.99	99.99	99.99	99.99	99.99

	HW_VOC_1000_2.5_4 MOLAR FRACTION OUT [%]					
T [K]	**1023**	**1043**	**1063**	**1083**	**1103**	**1123**
N2	7.87E+01	7.87E+01	7.87E+01	7.87E+01	7.88E+01	7.88E+01

O2	2.01E+01	2.00E+01	2.01E+01	2.01E+01	2.01E+01	2.01E+01
H2	1.07E-04	7.34E-05	4.86E-05	3.13E-05	2.04E-05	1.42E-05
H2O	4.73E-01	4.73E-01	4.71E-01	4.69E-01	4.66E-01	4.64E-01
CO	3.25E-02	2.27E-02	1.51E-02	9.63E-03	6.21E-03	4.27E-03
CO2	6.96E-01	7.04E-01	7.09E-01	7.10E-01	7.09E-01	7.08E-01
CH4	6.21E-05	4.29E-05	2.85E-05	1.83E-05	1.18E-05	8.09E-06
C3H6	4.84E-07	3.91E-07	2.86E-07	1.85E-07	1.13E-07	7.15E-08
C3H8	6.49E-13	2.86E-13	1.14E-13	4.05E-14	1.41E-14	5.50E-15
C2H2	3.54E-05	2.90E-05	2.34E-05	1.84E-05	1.41E-05	1.10E-05
C2H4	7.45E-05	5.86E-05	4.47E-05	3.25E-05	2.29E-05	1.64E-05
C2H6	7.64E-08	3.72E-08	1.66E-08	6.80E-09	2.71E-09	1.18E-09
CH2O	1.20E-04	8.80E-05	6.25E-05	4.28E-05	2.91E-05	2.06E-05
CH3OH	4.77E-05	3.37E-05	2.30E-05	1.53E-05	1.03E-05	7.20E-06
HCOOH	4.07E-06	2.85E-06	1.99E-06	1.39E-06	9.72E-07	7.00E-07
C7H8	1.36E-04	1.02E-04	7.39E-05	5.21E-05	3.64E-05	2.62E-05
C2H6O	9.91E-06	6.88E-06	4.60E-06	2.98E-06	1.95E-06	1.35E-06
Σ	99.99	99.99	99.99	99.99	99.99	99.99

HW_VOC_1000_10_1 MOLAR FRACTION OUT [%]

T [K]	1023	1043	1063	1083	1103	1123
N2	7.84E+01	7.84E+01	7.84E+01	7.84E+01	7.84E+01	7.84E+01
O2	1.91E+01	1.91E+01	1.91E+01	1.91E+01	1.91E+01	1.91E+01
H2	1.64E-04	1.08E-04	7.85E-05	6.14E-05	5.04E-05	4.28E-05
H2O	9.56E-01	9.53E-01	9.52E-01	9.51E-01	9.52E-01	9.53E-01
CO	2.81E-02	1.85E-02	1.33E-02	1.03E-02	8.41E-03	7.05E-03
CO2	1.47E+00	1.47E+00	1.48E+00	1.48E+00	1.48E+00	1.49E+00
CH4	9.65E-05	6.34E-05	4.54E-05	3.49E-05	2.81E-05	2.33E-05
C3H6	4.19E-07	2.54E-07	1.69E-07	1.22E-07	9.38E-08	7.43E-08
C3H8	1.00E-12	3.12E-13	1.21E-13	5.61E-14	2.92E-14	1.63E-14
C2H2	3.43E-05	2.55E-05	2.00E-05	1.65E-05	1.41E-05	1.24E-05
C2H4	1.08E-04	7.58E-05	5.63E-05	4.42E-05	3.61E-05	3.03E-05
C2H6	5.03E-08	1.80E-08	8.03E-09	4.29E-09	2.58E-09	1.68E-09
CH2O	1.04E-04	7.07E-05	5.20E-05	4.08E-05	3.34E-05	2.81E-05
CH3OH	5.30E-05	3.51E-05	2.52E-05	1.93E-05	1.54E-05	1.27E-05
HCOOH	1.14E-05	7.94E-06	5.84E-06	4.51E-06	3.58E-06	2.91E-06
C7H8	7.49E-05	5.29E-05	3.96E-05	3.13E-05	2.58E-05	2.17E-05
C2H6O	4.32E-06	2.87E-06	2.08E-06	1.62E-06	1.31E-06	1.09E-06
Σ	99.99	99.98	99.98	99.98	99.98	99.98

HW_VOC_1000_10_4 MOLAR FRACTION OUT [%]

T [K]	1023	1043	1063	1083	1103	1123
N2	7.84E+01	7.84E+01	7.84E+01	7.84E+01	7.84E+01	7.84E+01

O2	1.91E+01	1.91E+01	1.91E+01	1.91E+01	1.91E+01	1.91E+01
H2	3.88E-05	2.78E-05	2.16E-05	1.76E-05	1.49E-05	1.29E-05
H2O	9.58E-01	9.57E-01	9.57E-01	9.58E-01	9.60E-01	9.62E-01
CO	6.63E-03	4.73E-03	3.65E-03	2.96E-03	2.48E-03	2.11E-03
CO2	1.49E+00	1.49E+00	1.50E+00	1.50E+00	1.50E+00	1.51E+00
CH4	2.42E-05	1.70E-05	1.30E-05	1.04E-05	8.58E-06	7.22E-06
C3H6	4.84E-08	3.22E-08	2.36E-08	1.82E-08	1.45E-08	1.17E-08
C3H8	2.11E-14	8.31E-15	3.90E-15	2.04E-15	1.15E-15	6.83E-16
C2H2	1.01E-05	7.78E-06	6.37E-06	5.43E-06	4.75E-06	4.22E-06
C2H4	3.13E-05	2.26E-05	1.74E-05	1.41E-05	1.17E-05	9.86E-06
C2H6	2.91E-09	1.30E-09	6.93E-10	4.16E-10	2.69E-10	1.82E-10
CH2O	2.77E-05	1.99E-05	1.54E-05	1.25E-05	1.05E-05	8.93E-06
CH3OH	1.19E-05	8.55E-06	6.55E-06	5.23E-06	4.29E-06	3.58E-06
HCOOH	2.46E-06	1.80E-06	1.38E-06	1.09E-06	8.71E-07	7.06E-07
C7H8	2.10E-05	1.53E-05	1.19E-05	9.67E-06	8.06E-06	6.84E-06
C2H6O	1.02E-06	7.31E-07	5.63E-07	4.53E-07	3.74E-07	3.13E-07
Σ	99.99	99.98	99.98	99.99	99.99	99.99

HW_VOC_5000_2.5_1 MOLAR FRACTION OUT [%]

T [K]	**1023**	**1043**	**1063**	**1083**	**1103**	**1123**
N2	7.88E+01	7.88E+01	7.88E+01	7.88E+01	7.88E+01	7.88E+01
O2	2.04E+01	2.04E+01	2.04E+01	2.04E+01	2.04E+01	2.03E+01
H2	6.54E-04	4.99E-04	3.76E-04	2.77E-04	1.98E-04	1.36E-04
H2O	3.13E-01	3.21E-01	3.27E-01	3.31E-01	3.34E-01	3.35E-01
CO	2.24E-01	2.01E-01	1.76E-01	1.48E-01	1.19E-01	8.95E-02
CO2	2.49E-01	2.84E-01	3.19E-01	3.53E-01	3.87E-01	4.18E-01
CH4	3.09E-04	2.26E-04	1.62E-04	1.14E-04	7.72E-05	5.07E-05
C3H6	7.16E-06	7.04E-06	6.80E-06	6.38E-06	5.73E-06	4.82E-06
C3H8	2.80E-10	1.81E-10	1.11E-10	6.51E-11	3.55E-11	1.75E-11
C2H2	6.93E-04	5.42E-04	4.20E-04	3.23E-04	2.45E-04	1.83E-04
C2H4	5.01E-04	3.97E-04	3.12E-04	2.42E-04	1.84E-04	1.37E-04
C2H6	5.86E-06	4.02E-06	2.60E-06	1.57E-06	8.66E-07	4.26E-07
CH2O	1.45E-03	1.11E-03	8.43E-04	6.28E-04	4.58E-04	3.25E-04
CH3OH	6.48E-04	5.15E-04	4.05E-04	3.11E-04	2.31E-04	1.64E-04
HCOOH	2.50E-05	1.87E-05	1.38E-05	9.99E-06	7.14E-06	5.01E-06
C7H8	2.37E-03	1.75E-03	1.29E-03	9.40E-04	6.78E-04	4.82E-04
C2H6O	1.95E-04	1.50E-04	1.15E-04	8.59E-05	6.21E-05	4.31E-05
Σ	99.99	99.99	99.99	99.99	99.99	99.99

HW_VOC_1000_2.5_4 MOLAR FRACTION OUT [%]

T [K]	**1023**	**1043**	**1063**	**1083**	**1103**	**1123**
N2	7.88E+01	7.88E+01	7.88E+01	7.88E+01	7.88E+01	7.88E+01

O2	2.03E+01	2.03E+01	2.03E+01	2.03E+01	2.03E+01	2.03E+01
H2	1.71E-04	1.28E-04	9.40E-05	6.72E-05	4.68E-05	3.21E-05
H2O	3.35E-01	3.37E-01	3.38E-01	3.38E-01	3.37E-01	3.35E-01
CO	1.05E-01	8.54E-02	6.68E-02	4.97E-02	3.50E-02	2.37E-02
CO2	4.01E-01	4.25E-01	4.45E-01	4.62E-01	4.75E-01	4.82E-01
CH4	8.08E-05	5.85E-05	4.15E-05	2.87E-05	1.94E-05	1.29E-05
C3H6	2.39E-06	2.21E-06	1.99E-06	1.72E-06	1.38E-06	1.02E-06
C3H8	1.31E-11	7.66E-12	4.30E-12	2.26E-12	1.08E-12	4.62E-13
C2H2	1.73E-04	1.38E-04	1.09E-04	8.69E-05	6.86E-05	5.38E-05
C2H4	1.57E-04	1.26E-04	1.01E-04	8.00E-05	6.24E-05	4.78E-05
C2H6	7.42E-07	4.47E-07	2.55E-07	1.36E-07	6.69E-08	3.06E-08
CH2O	4.27E-04	3.29E-04	2.49E-04	1.85E-04	1.35E-04	9.71E-05
CH3OH	1.84E-04	1.42E-04	1.07E-04	7.82E-05	5.53E-05	3.82E-05
HCOOH	5.90E-06	4.23E-06	3.01E-06	2.13E-06	1.50E-06	1.06E-06
C7H8	6.31E-04	4.78E-04	3.60E-04	2.69E-04	1.98E-04	1.46E-04
C2H6O	5.45E-05	4.15E-05	3.08E-05	2.21E-05	1.53E-05	1.04E-05
Σ	99.99	99.99	99.99	99.99	99.99	99.99

HW_VOC_5000_10_1 MOLAR FRACTION OUT [%]

T [K]	**1023**	**1043**	**1063**	**1083**	**1103**	**1123**
N2	7.87E+01	7.87E+01	7.87E+01	7.87E+01	7.87E+01	7.87E+01
O2	2.03E+01	2.02E+01	2.02E+01	2.02E+01	2.02E+01	2.01E+01
H2	1.40E-03	1.04E-03	7.52E-04	5.27E-04	3.53E-04	2.29E-04
H2O	4.15E-01	4.23E-01	4.29E-01	4.32E-01	4.34E-01	4.33E-01
CO	2.66E-01	2.30E-01	1.91E-01	1.51E-01	1.11E-01	7.58E-02
CO2	3.73E-01	4.21E-01	4.68E-01	5.13E-01	5.55E-01	5.87E-01
CH4	7.61E-04	5.42E-04	3.79E-04	2.58E-04	1.69E-04	1.09E-04
C3H6	6.70E-06	6.49E-06	6.12E-06	5.51E-06	4.62E-06	3.51E-06
C3H8	5.65E-10	3.21E-10	1.70E-10	8.24E-11	3.54E-11	1.34E-11
C2H2	5.65E-04	4.29E-04	3.24E-04	2.41E-04	1.76E-04	1.27E-04
C2H4	7.10E-04	5.33E-04	3.98E-04	2.92E-04	2.10E-04	1.48E-04
C2H6	8.81E-06	5.60E-06	3.29E-06	1.75E-06	8.06E-07	3.24E-07
CH2O	1.39E-03	1.03E-03	7.52E-04	5.38E-04	3.74E-04	2.56E-04
CH3OH	7.09E-04	5.49E-04	4.17E-04	3.05E-04	2.12E-04	1.41E-04
HCOOH	7.87E-05	5.70E-05	4.07E-05	2.86E-05	1.97E-05	1.34E-05
C7H8	1.80E-03	1.29E-03	9.21E-04	6.52E-04	4.55E-04	3.17E-04
C2H6O	1.53E-04	1.15E-04	8.42E-05	5.98E-05	4.05E-05	2.65E-05
Σ	99.99	99.99	99.99	99.99	99.99	99.99

HW_VOC_5000_10_4 MOLAR FRACTION OUT [%]

T [K]	**1023**	**1043**	**1063**	**1083**	**1103**	**1123**
N2	7.87E+01	7.87E+01	7.88E+01	7.88E+01	7.88E+01	7.88E+01

O2	2.02E+01	2.01E+01	2.01E+01	2.01E+01	2.01E+01	2.01E+01
H2	3.58E-04	2.59E-04	1.82E-04	1.24E-04	8.21E-05	5.47E-05
H2O	4.35E-01	4.37E-01	4.37E-01	4.36E-01	4.33E-01	4.30E-01
CO	1.08E-01	8.35E-02	6.14E-02	4.27E-02	2.84E-02	1.87E-02
CO2	5.60E-01	5.86E-01	6.08E-01	6.25E-01	6.35E-01	6.39E-01
CH4	1.94E-04	1.38E-04	9.63E-05	6.52E-05	4.32E-05	2.87E-05
C3H6	2.08E-06	1.88E-06	1.62E-06	1.30E-06	9.45E-07	6.32E-07
C3H8	2.00E-11	1.02E-11	4.81E-12	2.07E-12	7.98E-13	2.88E-13
C2H2	1.38E-04	1.09E-04	8.57E-05	6.72E-05	5.21E-05	4.02E-05
C2H4	2.02E-04	1.58E-04	1.22E-04	9.26E-05	6.91E-05	5.08E-05
C2H6	9.32E-07	5.16E-07	2.64E-07	1.23E-07	5.20E-08	2.12E-08
CH2O	3.87E-04	2.91E-04	2.14E-04	1.55E-04	1.09E-04	7.69E-05
CH3OH	1.87E-04	1.40E-04	1.01E-04	7.05E-05	4.79E-05	3.24E-05
HCOOH	1.70E-05	1.20E-05	8.43E-06	5.90E-06	4.11E-06	2.88E-06
C7H8	4.65E-04	3.47E-04	2.58E-04	1.89E-04	1.37E-04	9.98E-05
C2H6O	4.01E-05	2.94E-05	2.09E-05	1.43E-05	9.56E-06	6.39E-06
Σ	99.99	99.99	99.99	99.99	99.99	99.99

Gas output

			HW_VOC_1000_2.5_1 GAS OUT			
T [K]	**1023**	**1043**	**1063**	**1083**	**1103**	**1123**
	[μg/h]	[μg/h]	[μg/h]	[μg/h]	[μg/h]	[μg/h]
H2	3.58E+05	2.56E+05	1.77E+05	1.19E+05	7.80E+04	5.21E+04
H2O	3.78E+09	3.79E+09	3.78E+09	3.77E+09	3.75E+09	3.72E+09
CO	1.35E+09	1.03E+09	7.42E+08	5.06E+08	3.32E+08	2.20E+08
CO2	1.21E+10	1.26E+10	1.30E+10	1.34E+10	1.35E+10	1.36E+10
CH4	1.56E+06	1.10E+06	7.59E+05	5.08E+05	3.34E+05	2.23E+05
C3H6	3.80E+04	3.40E+04	2.88E+04	2.24E+04	1.57E+04	1.03E+04
C3H8	4.27E-01	2.08E-01	9.37E-02	3.80E-02	1.38E-02	4.87E-03
C2H2	1.51E+06	1.19E+06	9.35E+05	7.28E+05	5.61E+05	4.31E+05
C2H4	2.66E+06	2.06E+06	1.57E+06	1.18E+06	8.72E+05	6.38E+05
C2H6	1.29E+04	6.94E+03	3.41E+03	1.52E+03	6.17E+02	2.48E+02
CH2O	5.05E+06	3.76E+06	2.75E+06	1.96E+06	1.37E+06	9.66E+05
CH3OH	2.68E+06	1.98E+06	1.41E+06	9.72E+05	6.53E+05	4.42E+05
HCOOH	3.99E+05	2.81E+05	1.96E+05	1.37E+05	9.51E+04	6.68E+04
C7H8	1.76E+07	1.31E+07	9.65E+06	7.04E+06	5.09E+06	3.69E+06
C2H6O	7.55E+05	5.47E+05	3.83E+05	2.59E+05	1.71E+05	1.15E+05

			HW_VOC_1000_2.5_2 GAS OUT			
T [K]	**1023**	**1043**	**1063**	**1083**	**1103**	**1123**
	[μg/h]	[μg/h]	[μg/h]	[μg/h]	[μg/h]	[μg/h]
H2	9.63E+04	6.62E+04	4.38E+04	2.82E+04	1.84E+04	1.28E+04
H2O	3.81E+09	3.81E+09	3.80E+09	3.78E+09	3.76E+09	3.74E+09
CO	4.08E+08	2.84E+08	1.89E+08	1.21E+08	7.78E+07	5.34E+07
CO2	1.37E+10	1.39E+10	1.40E+10	1.40E+10	1.39E+10	1.39E+10

CH4	4.45E+05	3.07E+05	2.04E+05	1.31E+05	8.49E+04	5.81E+04
C3H6	9.12E+03	7.35E+03	5.38E+03	3.49E+03	2.12E+03	1.35E+03
C3H8	1.28E-02	5.64E-03	2.24E-03	7.98E-04	2.78E-04	1.08E-04
C2H2	4.12E+05	3.37E+05	2.72E+05	2.14E+05	1.64E+05	1.28E+05
C2H4	9.35E+05	7.36E+05	5.61E+05	4.08E+05	2.87E+05	2.06E+05
C2H6	1.03E+03	5.00E+02	2.23E+02	9.14E+01	3.65E+01	1.59E+01
CH2O	1.61E+06	1.18E+06	8.39E+05	5.75E+05	3.91E+05	2.77E+05
CH3OH	6.84E+05	4.83E+05	3.30E+05	2.20E+05	1.47E+05	1.03E+05
HCOOH	8.39E+04	5.88E+04	4.10E+04	2.85E+04	2.00E+04	1.44E+04
C7H8	5.62E+06	4.19E+06	3.04E+06	2.15E+06	1.50E+06	1.08E+06
C2H6O	2.04E+05	1.42E+05	9.47E+04	6.14E+04	4.02E+04	2.79E+04

HW_VOC_1000_10_1 GAS OUT

T [K]	**1023**	**1043**	**1063**	**1083**	**1103**	**1123**
	[μg/h]	[μg/h]	[μg/h]	[μg/h]	[μg/h]	[μg/h]
H2	1.49E+05	9.80E+04	7.11E+04	5.56E+04	4.56E+04	3.87E+04
H2O	7.73E+09	7.71E+09	7.70E+09	7.70E+09	7.70E+09	7.71E+09
CO	3.53E+08	2.32E+08	1.67E+08	1.30E+08	1.06E+08	8.87E+07
CO2	2.90E+10	2.91E+10	2.92E+10	2.92E+10	2.93E+10	2.94E+10
CH4	6.95E+05	4.57E+05	3.27E+05	2.52E+05	2.03E+05	1.68E+05
C3H6	7.92E+03	4.79E+03	3.19E+03	2.31E+03	1.77E+03	1.40E+03
C3H8	1.99E-02	6.17E-03	2.40E-03	1.11E-03	5.78E-04	3.22E-04
C2H2	4.02E+05	2.99E+05	2.34E+05	1.93E+05	1.65E+05	1.45E+05
C2H4	1.37E+06	9.55E+05	7.10E+05	5.57E+05	4.55E+05	3.81E+05
C2H6	6.79E+02	2.43E+02	1.08E+02	5.80E+01	3.49E+01	2.27E+01
CH2O	1.40E+06	9.54E+05	7.02E+05	5.50E+05	4.50E+05	3.78E+05
CH3OH	7.62E+05	5.05E+05	3.63E+05	2.78E+05	2.22E+05	1.82E+05
HCOOH	2.36E+05	1.64E+05	1.21E+05	9.31E+04	7.41E+04	6.01E+04
C7H8	3.10E+06	2.19E+06	1.64E+06	1.30E+06	1.07E+06	8.98E+05
C2H6O	8.94E+04	5.95E+04	4.31E+04	3.34E+04	2.71E+04	2.25E+04

HW_VOC_1000_10_4 GAS OUT

T [K]	**1023**	**1043**	**1063**	**1083**	**1103**	**1123**
	[μg/h]	[μg/h]	[μg/h]	[μg/h]	[μg/h]	[μg/h]
H2	3.51E+04	2.52E+04	1.95E+04	1.60E+04	1.35E+04	1.17E+04
H2O	7.75E+09	7.74E+09	7.74E+09	7.75E+09	7.76E+09	7.78E+09
CO	8.35E+07	5.95E+07	4.59E+07	3.73E+07	3.12E+07	2.66E+07
CO2	2.95E+10	2.95E+10	2.96E+10	2.96E+10	2.97E+10	2.97E+10
CH4	1.74E+05	1.23E+05	9.35E+04	7.48E+04	6.18E+04	5.21E+04
C3H6	9.15E+02	6.08E+02	4.45E+02	3.44E+02	2.74E+02	2.20E+02
C3H8	4.18E-04	1.65E-04	7.72E-05	4.04E-05	2.27E-05	1.35E-05
C2H2	1.18E+05	9.10E+04	7.45E+04	6.35E+04	5.55E+04	4.94E+04
C2H4	3.94E+05	2.84E+05	2.19E+05	1.77E+05	1.47E+05	1.24E+05
C2H6	3.93E+01	1.75E+01	9.36E+00	5.62E+00	3.63E+00	2.45E+00
CH2O	3.73E+05	2.69E+05	2.08E+05	1.69E+05	1.41E+05	1.20E+05
CH3OH	1.72E+05	1.23E+05	9.42E+04	7.52E+04	6.17E+04	5.15E+04
HCOOH	5.08E+04	3.72E+04	2.85E+04	2.25E+04	1.80E+04	1.46E+04

C_7H_8	8.70E+05	6.34E+05	4.93E+05	4.00E+05	3.34E+05	2.83E+05
C_2H_6O	2.12E+04	1.51E+04	1.16E+04	9.37E+03	7.73E+03	6.47E+03

HW_VOC_5000_2.5_1 GAS OUT

T [K]	**1023**	**1043**	**1063**	**1083**	**1103**	**1123**
	[μg/h]	[μg/h]	[μg/h]	[μg/h]	[μg/h]	[μg/h]
H_2	2.95E+06	2.25E+06	1.69E+06	1.25E+06	8.90E+05	6.13E+05
H_2O	1.26E+10	1.29E+10	1.32E+10	1.33E+10	1.34E+10	1.35E+10
CO	1.40E+10	1.26E+10	1.10E+10	9.28E+09	7.45E+09	5.60E+09
CO_2	2.45E+10	2.80E+10	3.14E+10	3.48E+10	3.80E+10	4.10E+10
CH_4	1.11E+07	8.09E+06	5.81E+06	4.07E+06	2.77E+06	1.82E+06
C_3H_6	6.74E+05	6.63E+05	6.40E+05	6.00E+05	5.39E+05	4.53E+05
C_3H_8	2.76E+01	1.78E+01	1.10E+01	6.42E+00	3.49E+00	1.72E+00
C_2H_2	4.03E+07	3.15E+07	2.45E+07	1.88E+07	1.43E+07	1.06E+07
C_2H_4	3.14E+07	2.49E+07	1.96E+07	1.52E+07	1.15E+07	8.56E+06
C_2H_6	3.94E+05	2.70E+05	1.75E+05	1.05E+05	5.82E+04	2.86E+04
CH_2O	9.75E+07	7.47E+07	5.66E+07	4.22E+07	3.07E+07	2.18E+07
CH_3OH	4.64E+07	3.69E+07	2.90E+07	2.23E+07	1.65E+07	1.17E+07
HCOOH	2.57E+06	1.92E+06	1.41E+06	1.03E+06	7.34E+05	5.16E+05
C_7H_8	4.87E+08	3.60E+08	2.65E+08	1.94E+08	1.40E+08	9.93E+07
C_2H_6O	2.00E+07	1.55E+07	1.18E+07	8.85E+06	6.40E+06	4.44E+06

HW_VOC_5000_2.5_4 GAS OUT

T [K]	**1023**	**1043**	**1063**	**1083**	**1103**	**1123**
	[μg/h]	[μg/h]	[μg/h]	[μg/h]	[μg/h]	[μg/h]
H_2	7.71E+05	5.77E+05	4.23E+05	3.02E+05	2.11E+05	1.45E+05
H_2O	1.35E+10	1.36E+10	1.36E+10	1.36E+10	1.36E+10	1.35E+10
CO	6.57E+09	5.34E+09	4.18E+09	3.11E+09	2.19E+09	1.48E+09
CO_2	3.95E+10	4.18E+10	4.38E+10	4.54E+10	4.66E+10	4.74E+10
CH_4	2.90E+06	2.10E+06	1.49E+06	1.03E+06	6.94E+05	4.61E+05
C_3H_6	2.24E+05	2.08E+05	1.87E+05	1.61E+05	1.30E+05	9.56E+04
C_3H_8	1.29E+00	7.55E-01	4.23E-01	2.22E-01	1.06E-01	4.55E-02
C_2H_2	1.01E+07	8.00E+06	6.37E+06	5.05E+06	3.99E+06	3.13E+06
C_2H_4	9.82E+06	7.90E+06	6.32E+06	5.01E+06	3.91E+06	2.99E+06
C_2H_6	4.98E+04	3.00E+04	1.71E+04	9.12E+03	4.49E+03	2.05E+03
CH_2O	2.87E+07	2.20E+07	1.67E+07	1.24E+07	9.07E+06	6.51E+06
CH_3OH	1.31E+07	1.02E+07	7.66E+06	5.60E+06	3.96E+06	2.73E+06
HCOOH	6.07E+05	4.35E+05	3.10E+05	2.19E+05	1.55E+05	1.09E+05
C_7H_8	1.30E+08	9.84E+07	7.40E+07	5.53E+07	4.08E+07	3.00E+07
C_2H_6O	5.61E+06	4.27E+06	3.17E+06	2.27E+06	1.58E+06	1.07E+06

HW_VOC_5000_10_1 GAS OUT

T [K]	**1023**	**1043**	**1063**	**1083**	**1103**	**1123**
	[μg/h]	[μg/h]	[μg/h]	[μg/h]	[μg/h]	[μg/h]
H_2	6.32E+06	4.68E+06	3.39E+06	2.38E+06	1.59E+06	1.03E+06
H_2O	1.67E+10	1.71E+10	1.73E+10	1.74E+10	1.75E+10	1.74E+10
CO	1.67E+10	1.44E+10	1.20E+10	9.46E+09	6.94E+09	4.75E+09

CO_2	3.67E+10	4.15E+10	4.61E+10	5.05E+10	5.46E+10	5.78E+10
CH_4	2.73E+07	1.94E+07	1.36E+07	9.25E+06	6.07E+06	3.89E+06
C_3H_6	6.31E+05	6.11E+05	5.76E+05	5.18E+05	4.34E+05	3.30E+05
C_3H_8	5.58E+01	3.16E+01	1.68E+01	8.13E+00	3.49E+00	1.32E+00
C_2H_2	3.29E+07	2.50E+07	1.89E+07	1.40E+07	1.03E+07	7.42E+06
C_2H_4	4.46E+07	3.35E+07	2.50E+07	1.83E+07	1.32E+07	9.29E+06
C_2H_6	5.93E+05	3.77E+05	2.21E+05	1.17E+05	5.42E+04	2.18E+04
CH_2O	9.34E+07	6.91E+07	5.05E+07	3.61E+07	2.51E+07	1.72E+07
CH_3OH	5.09E+07	3.94E+07	2.99E+07	2.18E+07	1.52E+07	1.01E+07
HCOOH	8.11E+06	5.87E+06	4.19E+06	2.94E+06	2.03E+06	1.38E+06
C_7H_8	3.71E+08	2.66E+08	1.90E+08	1.34E+08	9.38E+07	6.53E+07
C_2H_6O	1.58E+07	1.18E+07	8.68E+06	6.16E+06	4.18E+06	2.73E+06

	HW_VOC_5000_10_4 GAS OUT					
T [K]	**1023**	**1043**	**1063**	**1083**	**1103**	**1123**
	[μg/h]	[μg/h]	[μg/h]	[μg/h]	[μg/h]	[μg/h]
H_2	1.61E+06	1.17E+06	8.21E+05	5.58E+05	3.70E+05	2.46E+05
H_2O	1.75E+10	1.76E+10	1.76E+10	1.75E+10	1.74E+10	1.73E+10
CO	6.77E+09	5.23E+09	3.85E+09	2.68E+09	1.78E+09	1.17E+09
CO_2	5.51E+10	5.77E+10	5.99E+10	6.15E+10	6.24E+10	6.29E+10
CH_4	6.96E+06	4.96E+06	3.45E+06	2.34E+06	1.55E+06	1.03E+06
C_3H_6	1.96E+05	1.77E+05	1.52E+05	1.22E+05	8.89E+04	5.94E+04
C_3H_8	1.97E+00	1.00E+00	4.74E-01	2.04E-01	7.87E-02	2.84E-02
C_2H_2	8.02E+06	6.33E+06	4.99E+06	3.91E+06	3.03E+06	2.34E+06
C_2H_4	1.27E+07	9.88E+06	7.63E+06	5.81E+06	4.33E+06	3.19E+06
C_2H_6	6.27E+04	3.47E+04	1.77E+04	8.24E+03	3.50E+03	1.43E+03
CH_2O	2.60E+07	1.95E+07	1.44E+07	1.04E+07	7.33E+06	5.16E+06
CH_3OH	1.34E+07	1.00E+07	7.24E+06	5.05E+06	3.43E+06	2.32E+06
HCOOH	1.75E+06	1.23E+06	8.68E+05	6.07E+05	4.23E+05	2.97E+05
C_7H_8	9.58E+07	7.16E+07	5.31E+07	3.90E+07	2.83E+07	2.05E+07
C_2H_6O	4.13E+06	3.03E+06	2.15E+06	1.48E+06	9.85E+05	6.58E+05

Weight By Weight Percentage Output

	HW_VOC_1000_2.5_1					
T[K]	**1023**	**1043**	**1063**	**1083**	**1103**	**1123**
	wt/wt% OUT	wt/wt% OUT	wt/wt% OUT	wt/wt% OUT	wt/wt% OUT	wt/wt% OUT
N_2	7.64E+01	7.64E+01	7.64E+01	7.64E+01	7.64E+01	7.64E+01
O_2	2.23E+01	2.22E+01	2.22E+01	2.22E+01	2.22E+01	2.22E+01
H_2	2.77E-05	1.98E-05	1.37E-05	9.19E-06	6.03E-06	4.03E-06
H_2O	2.92E-01	2.93E-01	2.93E-01	2.92E-01	2.90E-01	2.88E-01
CO	1.05E-01	7.97E-02	5.74E-02	3.92E-02	2.57E-02	1.70E-02
CO_2	9.35E-01	9.76E-01	1.01E+00	1.03E+00	1.05E+00	1.05E+00
CH_4	1.21E-04	8.52E-05	5.87E-05	3.93E-05	2.59E-05	1.72E-05
C_3H_6	2.94E-06	2.63E-06	2.23E-06	1.73E-06	1.22E-06	7.96E-07
C_3H_8	3.30E-11	1.61E-11	7.26E-12	2.94E-12	1.07E-12	3.77E-13

C2H2	1.17E-04	9.22E-05	7.24E-05	5.64E-05	4.34E-05	3.34E-05
C2H4	2.06E-04	1.59E-04	1.22E-04	9.17E-05	6.75E-05	4.94E-05
C2H6	1.00E-06	5.37E-07	2.64E-07	1.17E-07	4.77E-08	1.92E-08
CH2O	3.91E-04	2.91E-04	2.13E-04	1.52E-04	1.06E-04	7.48E-05
CH3OH	2.07E-04	1.53E-04	1.09E-04	7.53E-05	5.06E-05	3.42E-05
HCOOH	3.09E-05	2.17E-05	1.52E-05	1.06E-05	7.36E-06	5.17E-06
C7H8	1.36E-03	1.01E-03	7.47E-04	5.45E-04	3.94E-04	2.86E-04
C2H6O	5.84E-05	4.24E-05	2.97E-05	2.01E-05	1.33E-05	8.89E-06

HW_VOC_1000_2.5_4

T[K]	**1023**	**1043**	**1063**	**1083**	**1103**	**1123**
	wt/wt% OUT	wt/wt% OUT	wt/wt% OUT	wt/wt% OUT	wt/wt% OUT	wt/wt% OUT
N2	7.64E+01	7.64E+01	7.64E+01	7.64E+01	7.64E+01	7.64E+01
O2	2.22E+01	2.22E+01	2.22E+01	2.22E+01	2.22E+01	2.22E+01
H2	7.46E-06	5.13E-06	3.39E-06	2.19E-06	1.43E-06	9.90E-07
H2O	2.95E-01	2.95E-01	2.94E-01	2.92E-01	2.91E-01	2.90E-01
CO	3.16E-02	2.20E-02	1.46E-02	9.34E-03	6.02E-03	4.14E-03
CO2	1.06E+00	1.07E+00	1.08E+00	1.08E+00	1.08E+00	1.08E+00
CH4	3.45E-05	2.38E-05	1.58E-05	1.02E-05	6.57E-06	4.49E-06
C3H6	7.06E-07	5.69E-07	4.16E-07	2.70E-07	1.64E-07	1.04E-07
C3H8	9.91E-13	4.36E-13	1.73E-13	6.18E-14	2.15E-14	8.40E-15
C2H2	3.19E-05	2.61E-05	2.11E-05	1.66E-05	1.27E-05	9.92E-06
C2H4	7.24E-05	5.69E-05	4.35E-05	3.16E-05	2.22E-05	1.60E-05
C2H6	7.96E-08	3.87E-08	1.73E-08	7.08E-09	2.82E-09	1.23E-09
CH2O	1.25E-04	9.15E-05	6.49E-05	4.45E-05	3.03E-05	2.14E-05
CH3OH	5.29E-05	3.74E-05	2.55E-05	1.70E-05	1.14E-05	7.98E-06
HCOOH	6.49E-06	4.55E-06	3.18E-06	2.21E-06	1.55E-06	1.12E-06
C7H8	4.35E-04	3.24E-04	2.36E-04	1.66E-04	1.16E-04	8.36E-05
C2H6O	1.58E-05	1.10E-05	7.33E-06	4.76E-06	3.11E-06	2.16E-06

HW_VOC_1000_10_1

T[K]	**1023**	**1043**	**1063**	**1083**	**1103**	**1123**
	wt/wt% OUT	wt/wt% OUT	wt/wt% OUT	wt/wt% OUT	wt/wt% OUT	wt/wt% OUT
N2	7.59E+01	7.59E+01	7.59E+01	7.59E+01	7.59E+01	7.59E+01
O2	2.12E+01	2.12E+01	2.12E+01	2.12E+01	2.12E+01	2.12E+01
H2	1.14E-05	7.55E-06	5.47E-06	4.28E-06	3.51E-06	2.98E-06
H2O	5.95E-01	5.93E-01	5.93E-01	5.92E-01	5.93E-01	5.93E-01
CO	2.72E-02	1.79E-02	1.29E-02	1.00E-02	8.14E-03	6.83E-03
CO2	2.23E+00	2.24E+00	2.25E+00	2.25E+00	2.25E+00	2.26E+00
CH4	5.35E-05	3.52E-05	2.52E-05	1.94E-05	1.56E-05	1.29E-05
C3H6	6.10E-07	3.69E-07	2.45E-07	1.78E-07	1.36E-07	1.08E-07
C3H8	1.53E-12	4.75E-13	1.84E-13	8.56E-14	4.45E-14	2.48E-14
C2H2	3.09E-05	2.30E-05	1.80E-05	1.49E-05	1.27E-05	1.12E-05
C2H4	1.05E-04	7.35E-05	5.46E-05	4.29E-05	3.50E-05	2.93E-05

C2H6	5.23E-08	1.87E-08	8.35E-09	4.46E-09	2.69E-09	1.74E-09
CH2O	1.07E-04	7.34E-05	5.40E-05	4.23E-05	3.46E-05	2.91E-05
CH3OH	5.87E-05	3.89E-05	2.79E-05	2.14E-05	1.71E-05	1.40E-05
HCOOH	1.82E-05	1.26E-05	9.29E-06	7.17E-06	5.70E-06	4.63E-06
C7H8	2.39E-04	1.68E-04	1.26E-04	9.98E-05	8.20E-05	6.91E-05
C2H6O	6.88E-06	4.58E-06	3.32E-06	2.57E-06	2.08E-06	1.73E-06

			HW_VOC_1000_10_4			
T[K]	**1023**	**1043**	**1063**	**1083**	**1103**	**1123**
	wt/wt% OUT	wt/wt% OUT	wt/wt% OUT	wt/wt% OUT	wt/wt% OUT	wt/wt% OUT
N2	7.59E+01	7.59E+01	7.59E+01	7.59E+01	7.59E+01	7.59E+01
O2	2.11E+01	2.11E+01	2.11E+01	2.11E+01	2.11E+01	2.11E+01
H2	2.70E-06	1.94E-06	1.50E-06	1.23E-06	1.04E-06	9.00E-07
H2O	5.97E-01	5.96E-01	5.96E-01	5.97E-01	5.98E-01	5.99E-01
CO	6.42E-03	4.58E-03	3.54E-03	2.87E-03	2.40E-03	2.04E-03
CO2	2.27E+00	2.27E+00	2.27E+00	2.28E+00	2.28E+00	2.29E+00
CH4	1.34E-05	9.44E-06	7.20E-06	5.76E-06	4.76E-06	4.01E-06
C3H6	7.05E-08	4.68E-08	3.43E-08	2.65E-08	2.11E-08	1.70E-08
C3H8	3.22E-14	1.27E-14	5.94E-15	3.11E-15	1.75E-15	1.04E-15
C2H2	9.05E-06	7.00E-06	5.74E-06	4.89E-06	4.27E-06	3.80E-06
C2H4	3.04E-05	2.19E-05	1.69E-05	1.36E-05	1.13E-05	9.56E-06
C2H6	3.02E-09	1.35E-09	7.20E-10	4.33E-10	2.79E-10	1.89E-10
CH2O	2.87E-05	2.07E-05	1.60E-05	1.30E-05	1.09E-05	9.26E-06
CH3OH	1.32E-05	9.47E-06	7.25E-06	5.79E-06	4.75E-06	3.96E-06
HCOOH	3.91E-06	2.87E-06	2.19E-06	1.73E-06	1.39E-06	1.12E-06
C7H8	6.69E-05	4.88E-05	3.79E-05	3.08E-05	2.57E-05	2.18E-05
C2H6O	1.63E-06	1.16E-06	8.97E-07	7.21E-07	5.95E-07	4.98E-07

			HW_VOC_5000_2.5_1			
T[K]	**1023**	**1043**	**1063**	**1083**	**1103**	**1123**
	wt/wt% OUT	wt/wt% OUT	wt/wt% OUT	wt/wt% OUT	wt/wt% OUT	wt/wt% OUT
N2	7.65E+01	7.65E+01	7.65E+01	7.65E+01	7.65E+01	7.65E+01
O2	2.27E+01	2.26E+01	2.26E+01	2.26E+01	2.26E+01	2.25E+01
H2	4.57E-05	3.49E-05	2.63E-05	1.93E-05	1.38E-05	9.51E-06
H2O	1.96E-01	2.01E-01	2.04E-01	2.07E-01	2.09E-01	2.09E-01
CO	2.17E-01	1.95E-01	1.71E-01	1.44E-01	1.15E-01	8.68E-02
CO2	3.80E-01	4.34E-01	4.87E-01	5.39E-01	5.90E-01	6.37E-01
CH4	1.72E-04	1.25E-04	9.00E-05	6.31E-05	4.29E-05	2.82E-05
C3H6	1.05E-05	1.03E-05	9.92E-06	9.31E-06	8.36E-06	7.03E-06
C3H8	4.28E-10	2.77E-10	1.70E-10	9.95E-11	5.42E-11	2.67E-11
C2H2	6.25E-04	4.89E-04	3.79E-04	2.92E-04	2.21E-04	1.65E-04
C2H4	4.87E-04	3.86E-04	3.03E-04	2.35E-04	1.79E-04	1.33E-04
C2H6	6.10E-06	4.19E-06	2.71E-06	1.63E-06	9.02E-07	4.44E-07
CH2O	1.51E-03	1.16E-03	8.77E-04	6.54E-04	4.76E-04	3.38E-04

CH3OH	7.20E-04	5.72E-04	4.49E-04	3.45E-04	2.56E-04	1.82E-04
HCOOH	3.99E-05	2.98E-05	2.19E-05	1.59E-05	1.14E-05	8.00E-06
C7H8	7.56E-03	5.58E-03	4.11E-03	3.00E-03	2.17E-03	1.54E-03
C2H6O	3.11E-04	2.40E-04	1.83E-04	1.37E-04	9.92E-05	6.89E-05

			HW_VOC_5000_2.5_4			
T[K]	**1023**	**1043**	**1063**	**1083**	**1103**	**1123**
	wt/wt% OUT	wt/wt% OUT	wt/wt% OUT	wt/wt% OUT	wt/wt% OUT	wt/wt% OUT
N2	7.65E+01	7.65E+01	7.65E+01	7.65E+01	7.65E+01	7.65E+01
O2	2.26E+01	2.25E+01	2.25E+01	2.25E+01	2.25E+01	2.25E+01
H2	1.20E-05	8.95E-06	6.56E-06	4.69E-06	3.27E-06	2.24E-06
H2O	2.09E-01	2.10E-01	2.11E-01	2.11E-01	2.10E-01	2.09E-01
CO	1.02E-01	8.29E-02	6.48E-02	4.82E-02	3.40E-02	2.30E-02
CO2	6.12E-01	6.47E-01	6.79E-01	7.05E-01	7.23E-01	7.35E-01
CH4	4.49E-05	3.25E-05	2.30E-05	1.60E-05	1.08E-05	7.15E-06
C3H6	3.48E-06	3.23E-06	2.91E-06	2.50E-06	2.01E-06	1.48E-06
C3H8	2.00E-11	1.17E-11	6.56E-12	3.45E-12	1.65E-12	7.06E-13
C2H2	1.56E-04	1.24E-04	9.87E-05	7.84E-05	6.19E-05	4.85E-05
C2H4	1.52E-04	1.23E-04	9.81E-05	7.77E-05	6.06E-05	4.64E-05
C2H6	7.73E-07	4.65E-07	2.65E-07	1.41E-07	6.97E-08	3.19E-08
CH2O	4.45E-04	3.42E-04	2.59E-04	1.93E-04	1.41E-04	1.01E-04
CH3OH	2.04E-04	1.58E-04	1.19E-04	8.68E-05	6.13E-05	4.24E-05
HCOOH	9.41E-06	6.74E-06	4.80E-06	3.40E-06	2.40E-06	1.69E-06
C7H8	2.01E-03	1.53E-03	1.15E-03	8.57E-04	6.33E-04	4.65E-04
C2H6O	8.70E-05	6.63E-05	4.91E-05	3.52E-05	2.44E-05	1.66E-05

			HW_VOC_5000_10_1			
T[K]	**1023**	**1043**	**1063**	**1083**	**1103**	**1123**
	wt/wt% OUT	wt/wt% OUT	wt/wt% OUT	wt/wt% OUT	wt/wt% OUT	wt/wt% OUT
N2	7.64E+01	7.64E+01	7.64E+01	7.64E+01	7.64E+01	7.64E+01
O2	2.25E+01	2.24E+01	2.24E+01	2.24E+01	2.23E+01	2.23E+01
H2	9.79E-05	7.25E-05	5.25E-05	3.68E-05	2.47E-05	1.60E-05
H2O	2.59E-01	2.64E-01	2.68E-01	2.70E-01	2.71E-01	2.70E-01
CO	2.58E-01	2.23E-01	1.86E-01	1.46E-01	1.08E-01	7.36E-02
CO2	5.69E-01	6.42E-01	7.14E-01	7.82E-01	8.45E-01	8.95E-01
CH4	4.23E-04	3.01E-04	2.11E-04	1.43E-04	9.40E-05	6.03E-05
C3H6	9.77E-06	9.46E-06	8.92E-06	8.03E-06	6.73E-06	5.12E-06
C3H8	8.64E-10	4.90E-10	2.60E-10	1.26E-10	5.41E-11	2.05E-11
C2H2	5.10E-04	3.87E-04	2.92E-04	2.17E-04	1.59E-04	1.15E-04
C2H4	6.90E-04	5.19E-04	3.87E-04	2.84E-04	2.04E-04	1.44E-04
C2H6	9.18E-06	5.83E-06	3.43E-06	1.82E-06	8.39E-07	3.37E-07
CH2O	1.45E-03	1.07E-03	7.83E-04	5.60E-04	3.89E-04	2.66E-04
CH3OH	7.88E-04	6.10E-04	4.63E-04	3.38E-04	2.36E-04	1.57E-04
HCOOH	1.26E-04	9.09E-05	6.49E-05	4.56E-05	3.14E-05	2.14E-05

C7H8	5.74E-03	4.11E-03	2.94E-03	2.08E-03	1.45E-03	1.01E-03
C2H6O	2.45E-04	1.83E-04	1.34E-04	9.54E-05	6.47E-05	4.23E-05

	HW_VOC_5000_10_4					
T[K]	**1023**	**1043**	**1063**	**1083**	**1103**	**1123**
	wt/wt% OUT	wt/wt% OUT	wt/wt% OUT	wt/wt% OUT	wt/wt% OUT	wt/wt% OUT
N2	7.64E+01	7.64E+01	7.64E+01	7.64E+01	7.64E+01	7.64E+01
O2	2.23E+01	2.23E+01	2.23E+01	2.23E+01	2.23E+01	2.23E+01
H2	2.50E-05	1.81E-05	1.27E-05	8.64E-06	5.73E-06	3.82E-06
H2O	2.72E-01	2.72E-01	2.73E-01	2.72E-01	2.70E-01	2.68E-01
CO	1.05E-01	8.10E-02	5.96E-02	4.15E-02	2.76E-02	1.82E-02
CO2	8.53E-01	8.94E-01	9.27E-01	9.52E-01	9.67E-01	9.74E-01
CH4	1.08E-04	7.68E-05	5.35E-05	3.62E-05	2.40E-05	1.59E-05
C3H6	3.03E-06	2.74E-06	2.36E-06	1.89E-06	1.38E-06	9.20E-07
C3H8	3.05E-11	1.55E-11	7.35E-12	3.16E-12	1.22E-12	4.40E-13
C2H2	1.24E-04	9.80E-05	7.73E-05	6.06E-05	4.70E-05	3.62E-05
C2H4	1.97E-04	1.53E-04	1.18E-04	9.00E-05	6.71E-05	4.93E-05
C2H6	9.71E-07	5.37E-07	2.74E-07	1.28E-07	5.42E-08	2.21E-08
CH2O	4.02E-04	3.02E-04	2.23E-04	1.61E-04	1.14E-04	7.99E-05
CH3OH	2.07E-04	1.55E-04	1.12E-04	7.83E-05	5.31E-05	3.59E-05
HCOOH	2.71E-05	1.91E-05	1.34E-05	9.40E-06	6.55E-06	4.60E-06
C7H8	1.48E-03	1.11E-03	8.22E-04	6.04E-04	4.38E-04	3.18E-04
C2H6O	6.40E-05	4.70E-05	3.34E-05	2.29E-05	1.53E-05	1.02E-05

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