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CONCEPTS FOR THE USAGE OF ZEOLITIC MOLECULAR SIEVES IN FILTRATION PROCESSES

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Abstract: One of the most common processes using different types of zeolitic molecular sieves is the pressure-absorption PSA process, this process is used to separate a particular gas species from a gas mixture under pressure, depending on the molecular characteristics of the species and affinity for a specific adsorbent material. The paper presents a concept of using zeolitic molecular sieves in the air intake process of internal combustion engines. The concept is based on a study on the evolution of a number of parameters in the development of the various engines with which the VW Golf model was equipped in the period 1974-2004. Implementation of the concept aims to reduce the air mass flow into the engine without adversely affecting its performance. In the study were analyzed a number of factors such as the evolution of cylindrical capacities for diesel engines, evolution of the mass of the vehicle, intake air mass flow rate and the amount of fuel consumed. Analysis of the data collected shows a steady increase of the cylinder capacity which can be attributed to the request of a more powerful engine units, demand that came from the market.
Keywords: molecular sieves, zolites, molecular filtration, internal combustion engines

1. INTRODUCTION

Molecular sieves are uniform pore materials, pore diameters are similar to the size of the small molecules which make it possible to filter or absorb them. As a mixture of molecules migrate through the stationary bed of porous material called the sieve, molecular components with the highest molecular weight (which are unable to pass through the molecular pores) leave the first bed by successive smaller molecules. Molecular sieve pore diameters are measured in ångströms (Å) or nanometers (nm), according to IUPAC (International Union of pure and applied Chemistry), porous materials having pore diameters less than 2 nm (20 Å) may be called micro-porous materials, and the macro-porous materials are those having pore diameters greater than 50 nm (500 Å), pore diameter materials between 50 nm (500 Å) being considered as mesoporous. Of the most common micro-porous materials used in the form of a molecular site we can mention: Zeolites, active Carbon, Monmonirolite or porous glass. [1]

The classification of the types of microporous molecular sieves is made on the basis of the diameter of the micro porosity that they have, in table 1 being presented the most common types of microporous sieves.

Table 1. Classification of microporous molecular sieves

Model	Pore diameter (Ångström)	Water absorption capacity (% of own mass)	Specific density (G / ml)
3Å	3	19–20	0.60–0.68
4Å	4	20–21	0.60–0.65
5Å-DW	5	21–22	0.45–0.50
5Å small	5	≥23	0.4–0.8
5Å	5	20–21	0.60–0.65
10X	8	23–24	0.50–0.60
13X	10	23–24	0.55–0.65
13X-AS	10	23–24	0.55–0.65
Cu-13X	10	23–24	0.50–0.60

- **Molecular sieves 3Å** with the chemical formula $((K_2O)_{2/3}\ (Na_2O)_{1/3})\cdot Al_2O_3\cdot 2\ SiO_2\cdot\ 9/2\ H_2O$ have an aluminum silico ratio of ≈2, because of the pore diameter of 3Å they do not adsorb larger molecules. This type of molecular sieve has several characteristics which lead to an improvement in the efficiency and also at a high lifetime, fast adsorption speed, frequent regeneration capacity, and good mechanical crushing resistance. Molecular sieves 3 Å are required in the oil and chemical industries for oil refining, polymerization and chemical drying.
- **Molecular sieves 4Å** with the chemical formula $Na_2O\cdot Al_2O_3\cdot 2SiO_2\cdot 9/2H_2O$ with an alumina silico ratio of ≈2, is widely used for drying laboratory solvents. They can absorb water and other molecules with a critical diameter of less than 4 Å such as NH_3, H_2S, SO_2, CO_2, C_2H_5OH, C2H6 and C_2H_4. Molecular sieves of type

4Å are being used in the production of detergents, due to a special feature which by exchange of calcium ions they will facilitate the production of demineralized water. It can also be used as a soap-forming agent or can be found in toothpaste.

≡ **Molecular sieves 5Å** with the chemical formula $0.7CaO \cdot 0.3Na_2O \cdot Al_2O_3 \cdot 2.SiO_2 \cdot 4.5H_2O$ have an alumina silico ratio of ≈2. They are used for drying natural gas together with performing desulfurization and decarbonization of gases. They can also be used to separate the mixtures of oxygen, nitrogen, hydrogen and hydrocarbons from branched and polycyclic hydrocarbons.

Alumino-silates of calcium, strontium, sodium, potassium, barium, magnesium are called zeolites. These may be natural or synthetic. They are characterized by a cube structure in the form of a honeycomb with and surrounded by 4 oxygen atoms. They belong together with feldspar to the group of tectosilicates. Zeolites have structures that are much more open and less dense than other silicates. Zeolites are negatively charged rare minerals, uniquely propagate in the mineral category. [2]

The porous structure of zeolites creates a large specific surface which gives them the character of absorbents, the access of molecules to the absorption surface being possible only through the hexagonal "windows" (Figure 1) of the sodium unit, conferring by the geometrical selectivity process the molecular sieve property (Figure 2).

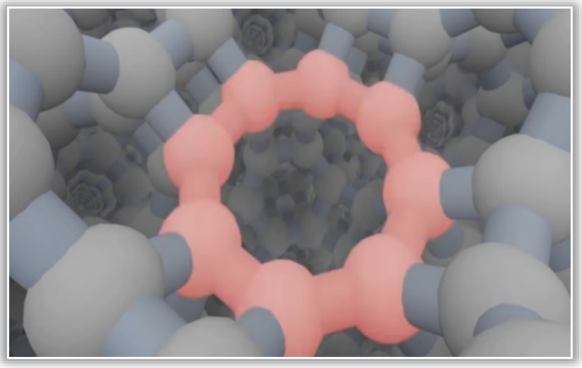

Figure 1 .Schematic representation of a hexagonal window

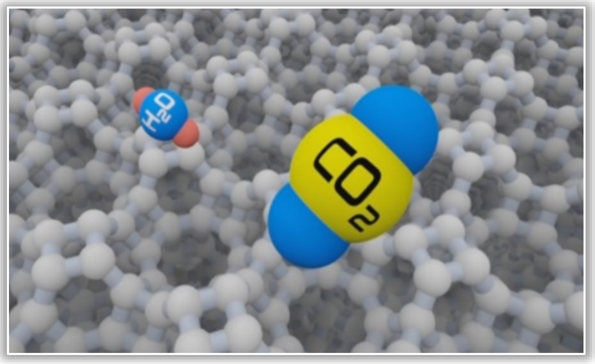

Figure 2. Schematic representation of geometric selectivity

At the porous level, zeolite have a particular structure, while in most of the absorbents material the parametric distribution has a Gaussian shape over a relative large range of pore diameter, in the case of zeolites the distribution curve has so narrow limits that it can be reduced to a straight line (Figure 3) [3].

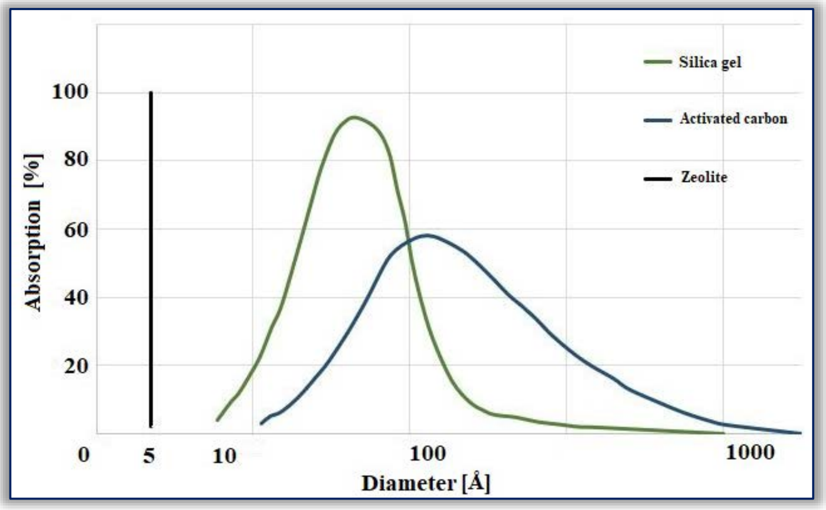

Figure 3. Distribution of pores in the case of zeolite as compared with silica gel and activated carbon [3]

One of the most common processes using different types of zeolitic molecular sieves is the pressure-absorption PSA process, this process is used to separate a particular gas species from a gas mixture under pressure, depending on the molecular characteristics of the species and affinity for a specific adsorbent material. This process operates at ambient temperatures and presents significantly differences from cryogenic distillation techniques. The adsorbent materials used such as activated carbon or zeolitic molecular sieves are used as absorbent for the target gases and then at low pressure they are extracted from the absorbent material. This process is also used for medical oxygen concentrates, in some cases the result is a gas with 90 % concentration of oxygen. [4]

2. CONCEPTUAL ANALYSIS REGARDING INTEGRATION OF MOLECULAR SIEVES INTO THE INTAKE SYSTEM OF INTERNAL COMBUSTION ENGINES

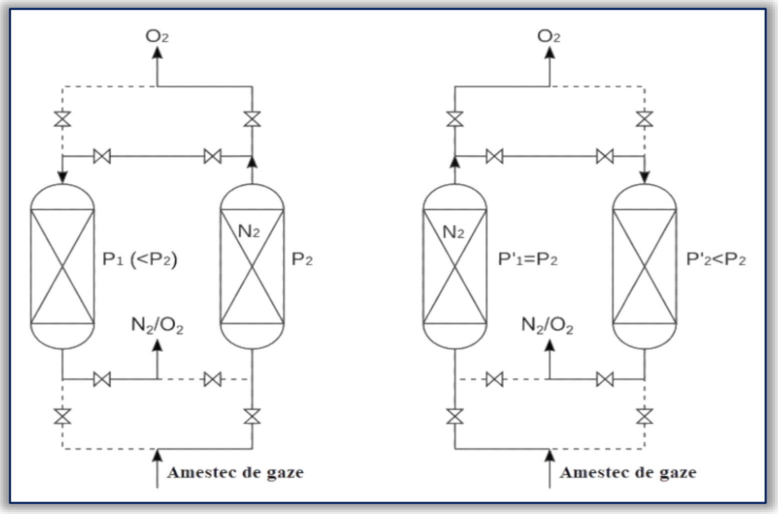

Figure 4. Schematic representation of the pressure absorption process [4]

In the case of internal combustion engines aspirated the intake gases are trapped inside the engine by atmospheric pressure which fills the volumetric gap caused by the down stroke of the piston. The ratio of the quantity of air admitted to the quantity of theoretical air obtained at ideal conditions is called volumetric efficiency. In order to achieve a high efficiency, the maximum volumetric efficiency is desired, the turbocharger was used for the first time in 1915. This device uses the energy from the exhaust of the flue gas to compress the air intake into the cylinders. As the compression process of fresh air increases internal energy, gas temperatures increase, thus decreasing their density. In this sense modern supercharger installations have a radiator, called intercooler, which is designed to lower the air temperature and increase its density, so that a higher mass flow of oxygen will be admitted in the same volume of the engine cylinders. Analysing the pressure absorption process described in the previous chapter we can see that a single passage of air through the molecular sieve is needed to obtain a volume of gas with a high oxygen concentration. This part of the process can also be implemented in the intake system of internal combustion engines. [5]

The results of the study that demonstrate the need to develop a more efficient method of oxygen concentration enrichment for the intake gases are presented in Figure 5.

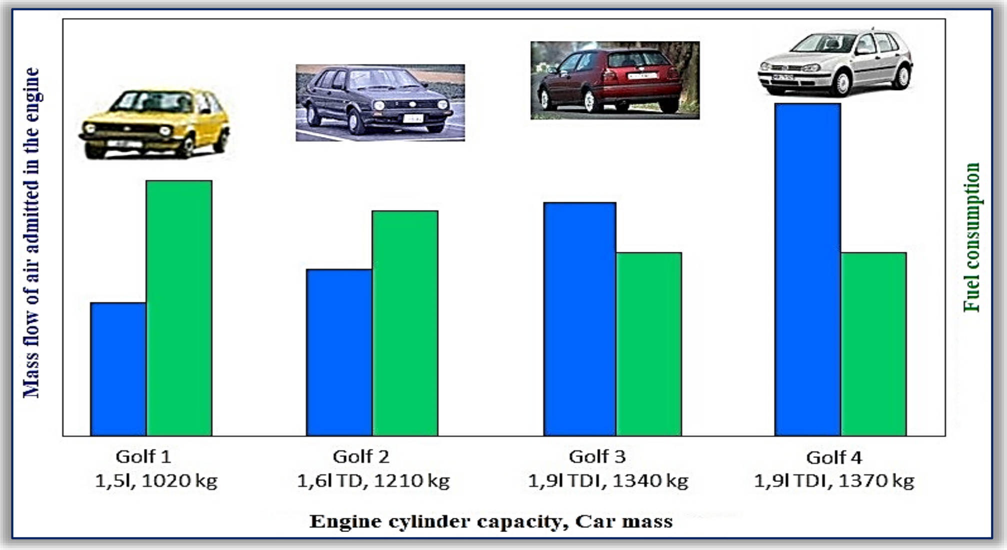

Figure 5. Analysis of the development direction of the last 25 years of the VW Golf model

In the study were analyzed a number of factors such as:

- the evolution of cylindrical capacities for diesel engines;
- evolution of the mass of the vehicle;
- intake air mass flow rate;
- the amount of fuel consumed;

Analysis of the data collected shows a steady increase of the cylinder capacity which can be attributed to the request of a more powerful engine units, demand that came from the market. However, with the increased cylinder capacity, the air mass flow it was doubled, which has increased the pressure drop along the inlet circuit route and also increased quantities of particles in suspension that required filtration. At the same time, we can see that, contrary to expectations, fuel consumption has fallen by about 25%. The increase in performance, which is linked to a decrease in fuel consumption, is due to the continues improvements of the injection systems, and the increased injection pressures, which has made possible to obtain a homogeneous fuel mixture.

3. CONCLUSIONS

In conclusion, if we consider an air component as follows: N_2 – 78% O_2 – 21% and 1% other gases, by integrating a molecular site module that would retain part of the nitrogen contained in this gas mixture admitted to the engine, we could increase the oxygen concentration to 42%. This would result in a mass flow reduction of 50%. Also due to decreased admitted volumetric flow rate, the engine cylindrical capacity can be reduced while keeping the same energetic level produced. Successful implementation of this concept could support the concept of downscaling which underpins the R&D processes of the modern car industry.

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