# USING ACTIVATED CARBON & CO EFFICIENTLY

The extraction of gas molecules from a gas mixture and their adsorption onto a solid plays an important role in many industrial processes. In many cases, technical systems are used today for these adsorption processes that are oversized for their task. This consumes unnecessarily high amounts of adsorption materials, investment resources and energy. To avoid this, a team of researchers from the Lucerne University of Applied Sciences and Arts has developed a model and an associated guideline. They help process engineers to better design the appropriate dimensions of gas purification and gas recovery plants in proportion with requirements. The scientists estimate the potential energy savings at 25 to 30 percent.



Adsorption processes have long played an important role in industry. A more recent application example is the process for CO<sub>2</sub> capture from the atmosphere, as offered by the Zurich-based company Climeworks. Photo: Julia Dunlop/Climeworks

A technical report about the results of several research projects in the field of industrial processes, which were financially supported by the Swiss Federal Office of Energy. The report has been published in the technical magazine ChemieXtra (issue September 2021).



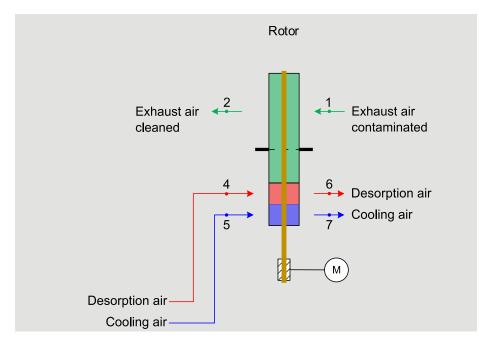
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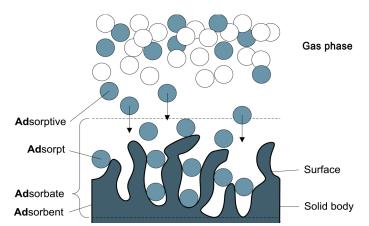
Cleaning solvents from the air of a paint shop, drying of gas mixtures in the plant of a cryogenic liquid manufacturer, or removing ammonia from the air of a livestock farm, all use the process of adsorption to remove a substance from a gas mixture. In these and many other processes, the substance attaches itself onto a solid (adsorbent) and is later separated from it in concentrated form and disposed of or reused. Adsorption processes not only provide valuable services in industry, but also in building technology: In air conditioning systems, the process is used to dehumidify the air and remove odorous substances. Similarly, in stove hoods, an activated carbon filter binds kitchen odours.

Adsorption processes have wide application in the chemical industry, in the separation of gas mixtures in refineries, for example, or the recovery of nitrogen and oxygen. They are also used in the food industry. The adsorption of gases is also of great importance in environmental and energy technology. One example is the separation of  $CO_2$  for refining raw biogas or the removal of dioxins or mercury from exhaust gases. A relatively new process is the capture of  $CO_2$  from the air in order to counteract climate change. The carbon dioxide obtained in this way can be used by the chemical industry, for example, instead of using 'technical  $CO_2$ ,' which must be specifically produced.

#### **Correctly Sizing Facilities**

Although adsorbers have been widely used in industry for a long time, there is often considerable potential for improve-





Schematic representation of an adsorption process from the gas phase: The gas mixture consists of two types of molecules (light and dark spheres). One molecule is taken up by the surface structures of the adsorbent. Illustration: Guide EESP

ment in their use. "Today, adsorbers that are oversized for their task are often used and have very high safety margins. This not only causes excessive investment costs, but also gobbles up an unnecessary amount of energy during operation," says Prof. Mirko Kleingries, a trained mechanical engineer with industrial experience who now heads the 'Thermal Energy Systems and Process Engineering' competence center at the Lucerne University of Applied Sciences and Arts.

Kleingries is part of an HSLU research team that has been studying adsorption processes for years with a view to their potential applications and optimization. For example, the study 'Technical Sorption Processes for Energy Applications' (TSEA),

> Schematic representation of an adsorption rotor that removes unwanted odorants from the exhaust air in an industrial plant: The rotor consists of a cylinder (shown here simplified as a greenred-blue rectangle) that is set in rotation by a motor (M). The rotor has a honeycomb structure on its surface. This structure absorbs the odour molecules contained in the exhaust air. In a second sub-process, the accumulated odour molecules are separated from the rotor and disposed of; the separation is achieved by flowing desorption air (here consisting of a hot air stream) and cool air through the rotor. Illustration: Guide EESP

I	Task	Create an overview of the task
	As-is analysis	Create overview of existing infrastructure, record process boundary conditions, record available energies (electricity, waste heat, etc.)
	▼ Target functions	Definition of one or more weighted target functions
IV	▼ Sorbent selection	Selection of the sorbent based on literature, manufacturer's specifications, design guidelines
V	▼ Process definition	Definition of process control, adsorber design, desorption process, etc.
VI	Model creation	Creation of a mathematical model, preferably with 1D-base module from SYSKON
	•	
VII	Model validation	Model validation on the basis of a reference case, if necessary carrying out of experimental investigations
	•	
VIII	Sensitivity analysis	Determine the influential parameters using an automated sensitivity analysis
	•	
IX	Optimization	Conduct parameter studies to best resolve conflicting objectives
	•	
x	Fine design	Fine design of the plant, again possible with 1D-base module

In order to optimally design adsorption processes from the gas phase, HSLU researchers have developed a guideline with ten steps. Illustration: Guide EESP

which was funded by the SFOE, was conducted in 2014-16. The study found considerable energy-savings potential in sorption processes, which can contribute to savings in the Energy Strategy 2050 in the area of industrial processes.

#### **Guideline Allows Structured Planning**

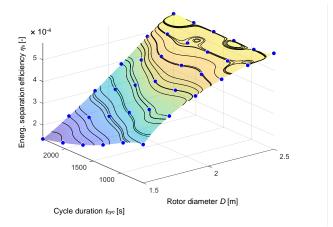
Against this background, researchers led by Mirko Kleingries have been looking for ways to realize this savings potential in recent years. In the SFOE project SYSKON, they developed a mathematical-physical model to describe adsorption processes in which a substance from a gas mixture is attached to a solid. For the most recent project, called EESP (acronym for the German: 'Empfehlungen zum Energieeffizienten Einsatz von Adsorptionsprozessen aus der Gasphase'), they developed a guideline that chemical and process engineers can use to plan and correctly dimension adsorption plants.

The design of adsorption processes is complex because a large number of influencing variables have to be taken into account. "With our guideline, we want to offer a structured approach to enable optimal plant design," says Kleingries. The guide comprises ten steps. These include the definition of the (e.g. economic or energetic) goals to be achieved with the respective adsorption process, but also sequential steps for technical implementation (see text box on the left).

#### **Robust and Sufficiently Accurate**

A central step is the creation of a mathematical-physical model that describes the adsorption process quantitatively. For this purpose, a software tool can be used that the scientists had developed in the precursor project SYSKON. "The model captures all relevant interactions of the adsorption process with sufficient accuracy, and at the same time the model is fast and robust," says Prof. Dr. Ulf Christian Müller, who teaches at the HSLU Competence Center in the field of fluid mechanics and thermodynamics. "Compared to tools available on the market, which are often very sophisticated and inflexible, our tool can be adapted to a wide range of use cases with relatively small effort thanks to its modular structure," Müller says.

After validation, the model can be used for sensitivity analysis and optimization of the adsorption process at hand. However, the model is not designed for the fine design of the plant—the last of the ten steps in the guide. "Anyone who follows our guide avoids oversizing their adsorption plant and thus escapes a danger that we have often observed in practice," says Müller. Based on two practical examples, Mül-



This diagram illustrates three important parameters of gas purification by adsorption. From the diagram one can see, for example, that the rotor diameter in this example must be chosen as large as possible and the cycle duration as short as possible in order to achieve a high energetic separation efficiency. The desired objectives can be achieved by suitable mathematical analysis (Pareto-optimization). Illustration: Final report EESP ler estimates the energy savings from correct dimensioning at 25 to 30 %. In the future, the HSLU scientists want to demonstrate that such efficiency increases can also be implemented in practice with applications of their modeling tool in industrial practice.

The final report of the project (Empfehlungen zum Energieeffizienten Einsatz von Adsorptionsprozessen aus der Gasphase) (EESP) and the (Leitfaden zur systematischen Auslegung technischer Adsorptionsprozesse aus der Gasphase) are available at: www.aramis.admin.ch/Texte/?ProjectID=47440. The final report of the project (Systematische Konzipierung industrieller Ad- und Desorptionsprozesse) (SYSKON), in which the model has been developed, is available at: www.aramis.admin.ch/Texte/?ProjectID=40680. A preliminary study around sorption processes under the name (Technische Sorptionsprozesse für energetische Anwendungen) (TSEA) is available at: www.aramis.admin.ch/Texte/?ProjectID=35930.

Support for the implementation of an industrial adsorption process using the software mentioned in the main text is provided by HSLU researcher Prof. Dr. Mirko Kleingries (mirko.kleingries[at]hslu.ch), Head of the Competence Center 'Thermal Energy Systems and Process Engineering' as well as by Prof. Dr. Ulf Christian Müller (ulfchristian.mueller[at]hslu.ch), Lecturer at the HSLU Competence Center 'Fluid Mechanics and Numerical Methods'.

## TEN STEPS TO THE GOAL

The guideline developed by researchers at the Lucerne University of Applied Sciences and Arts enables a systematic approach to the design of adsorption processes from the gas phase. The ten steps are summarized below:

Task definition: The core task of the process is defined.

**As-is analysis**: All available process data (such as temperature levels, gas volume flows, pressures and ambient conditions) are collected, process control parameters are determined and the space available for the plant is clarified. Attention is given to available energies (waste heat, process steam, etc.).

**Target functions**: Determination of the goals to be achieved by the adsorption process (e.g., low process costs, low energy consumption).

**Sorbent selection**: Determination of the adsorbent that optimally fulfills the application at hand (with reference to the equilibrium and kinetics data, the accuracy of which is of elementary importance).

**Process definition**: Determination of the process control and the design of the adsorption equipment including the associated desorption process (for example by means of temperature swing and/or pressure swing desorption).

**Model creation**: Creation of a mathematical-physical model to describe the adsorption process, for which the researchers at the Lucerne University of Applied Sciences and Arts have developed a basic model in the Modelica modeling language. By combining several basic modules, a variety of adsorber types can be modeled.

**Model validation**: The model is validated using reference cases from the literature with adapted boundary conditions or using measured data. Important parameters concern process equilibrium and kinetics, mass and heat transfer.

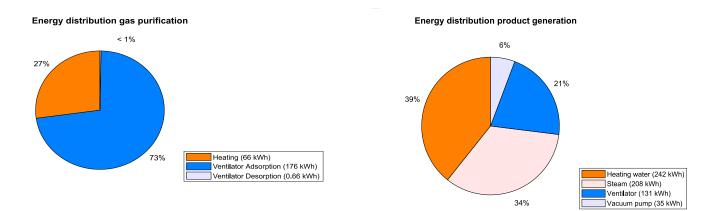
**Sensitivity analysis**: All parameters of the plant are varied and the possible operating points are shown in a main effect diagram and an interaction diagram. In this way, the parameters with the greatest influence on the optimal target function(s) and their interaction are determined ('Design of Experiment'/DoE).

**Optimization**: Based on the previous step, mathematical methods are used to determine how best to achieve the optimal target function(s).

**Fine design**: The final step is the fine design of the adsorption plant (the Modelica software mentioned above is not designed for fine design of the plant).

With the guide and the software tool, the two central tools are ready for practical use. The tool has been tested and validated for the two most important adsorber types - fixed bed and rotor adsorbers. BV

### 5 .....Using Activated Carbon & Co Efficiently



Two important applications of adsorption processes are the purification of unwanted gases from gas mixtures and the recovery of a substance from a gas mixture. The graphs show the energy breakdown for examples of the two process types: In the case of gas purification, about threequarters of the energy is used to power the fan that moves the gas mixture through the adsorber. About one quarter of the energy is required for heating the desorption air, which dissolves the substance molecules adhering to the adsorber. The energy requirement is distributed quite differently in the example from product recovery: Here, a lot of thermal energy is required to produce hot water and steam and only just under a quarter is required for the electric drive of the fan. The differences in energy requirements mean that the two applications require different efficiency measures. Illustrations: Final report EESP

- For information on the research projects, please contact Dr. Carina Alles (<u>carina.alles[at]bfe.admin.ch</u>), Head of the SFOE Research Program Industrial Processes.
- Further technical papers on research, pilot, demonstration and flagship projects in the field of industrial processes can be found at www.bfe.admin.ch/ec-prozesse.

## A LOT OF CHOICE

In order to adsorb certain substances from a gas mixture, thousands and thousands of adsorption materials ('adsorbents') are available today. These can be grouped according to their basic materials into carbonaceous adsorbents (e.g. activated carbon), oxidic adsorbents (e.g. zeolites or silica gel) and polymer adsorbents. All these adsorbent materials have different properties and are used for different purposes.

In addition to being widely used in industrial processes, adsorbent materials are also used in households. For example, steam extraction hoods in kitchens usually use activated carbon to remove unwanted odors from the exhaust air. Another application is packets of small beads, which are often enclosed in packaging. The silica gel beads ensure that the air is dried, thus preventing moisture from affecting the packaged goods. BV