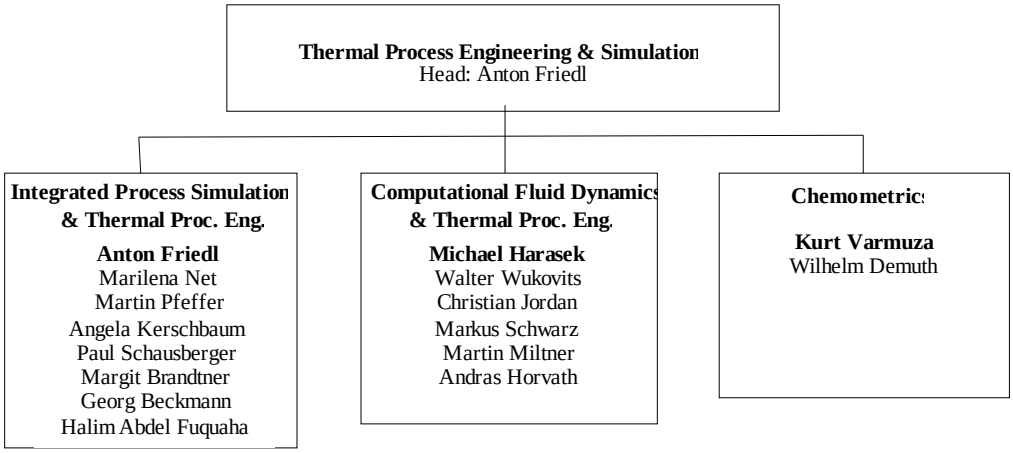
2. THERMAL PROCESS ENGINEERING



RESEARCH GOALS:

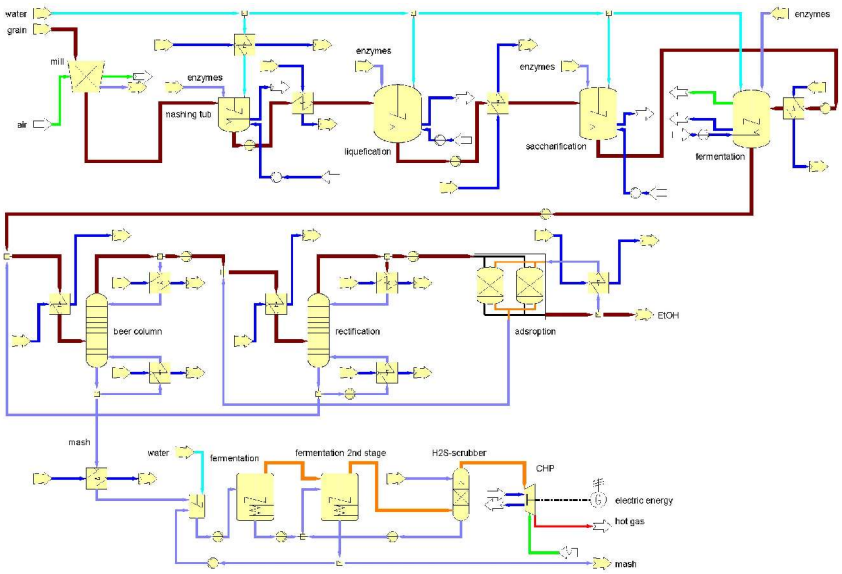
- Thermal Process Engineering (Membrane processes, Adsorption, Drying)
- Chemical, biotechnological and environmental applications of separation processes
- Process simulation (Chemical Engineering, Bioprocess Engineering, Energy Technology)
- Computational fluid dynamics (Process Engineering, Energy Technology)
- Chemometrics, Chemoinformatics

2.1 Process Simulation & Thermal Process Engineering

ETHANOL PRODUCTION COUPLED WITH A BIOENERGY PRODUCTION PLANT

Ethanol production from agricultural feedstock by fermentation is a well known process. In the last few years a growing importance of ethanol in the area of liquid fuel can be observed. This importance is strengthened by the increasing oil price as well as the growing awareness on CO_2-neutrality. In this context the European Union recommends that 2005 2% and 2010 5,75% of the demand on liquid fuel should come from renewable sources. To meet this guideline, besides the production of bio-diesel, also the production of bio-ethanol has to be increased.

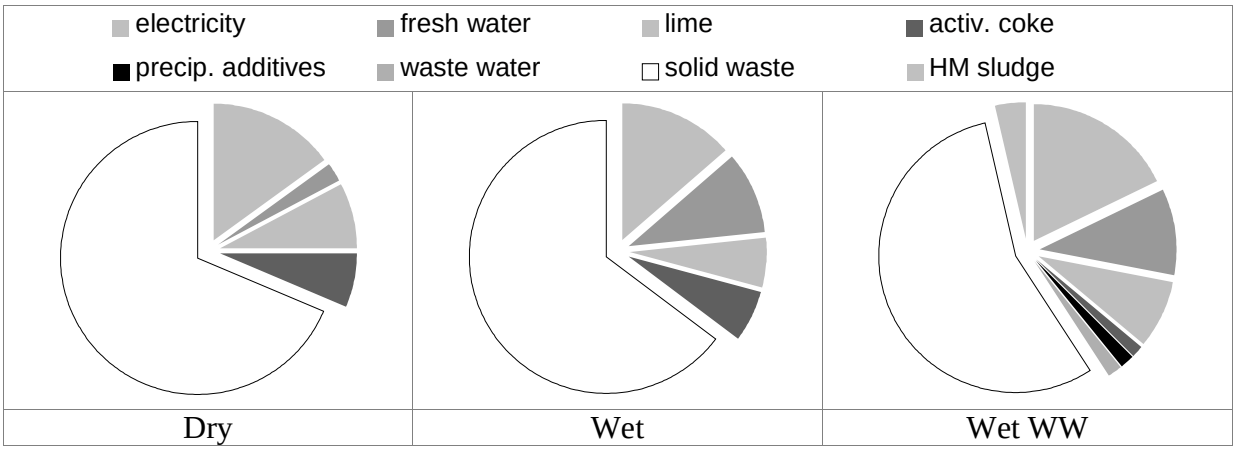
The economic validity of the ethanol production process depends on the amounts of used energy. To increase the economic efficiency of ethanol as liquid fuel compared to the fuel production from oil, a number of optimization steps had been proposed concerning the purification of ethanol, because especially concentration and dewatering of ethanol by distillation needs high energy requirements. In this context the aim of the project is a hundred percent supply of a local region with renewable energy. To reach this aim the integration of an ethanol plant in an existing network of biomass production facilities for heat and power is investigated by using process simulation and the industrial software package IPSEpro is used. IPSEpro and its commercialized standard unit library (APP_LIB) provides a base for the development for the required units as well as the needed substance data for ethanol, the desired enzymes and catalysts and the used biomass. The process model includes standard units like fermentation, distillation and adsorption as well as product separation using membrane processes.



This all results in a feasibility study of the implementation of an ethanol production plant from agricultural feedstock with special attention to the implementation of the ethanol production in an environment of existing production facilities for heat and energy. The extension of the commercialized simulation tool enables a calculation of production facilities for biomass conversion to heat, electric power and fuel as well as process optimization including new separation units. FFF-EdZ-Projekt: 807764 TU-Wien, Energiepark Bruck/Leitha

PROCESSSIMULATION: FLUEGAS CLEANING

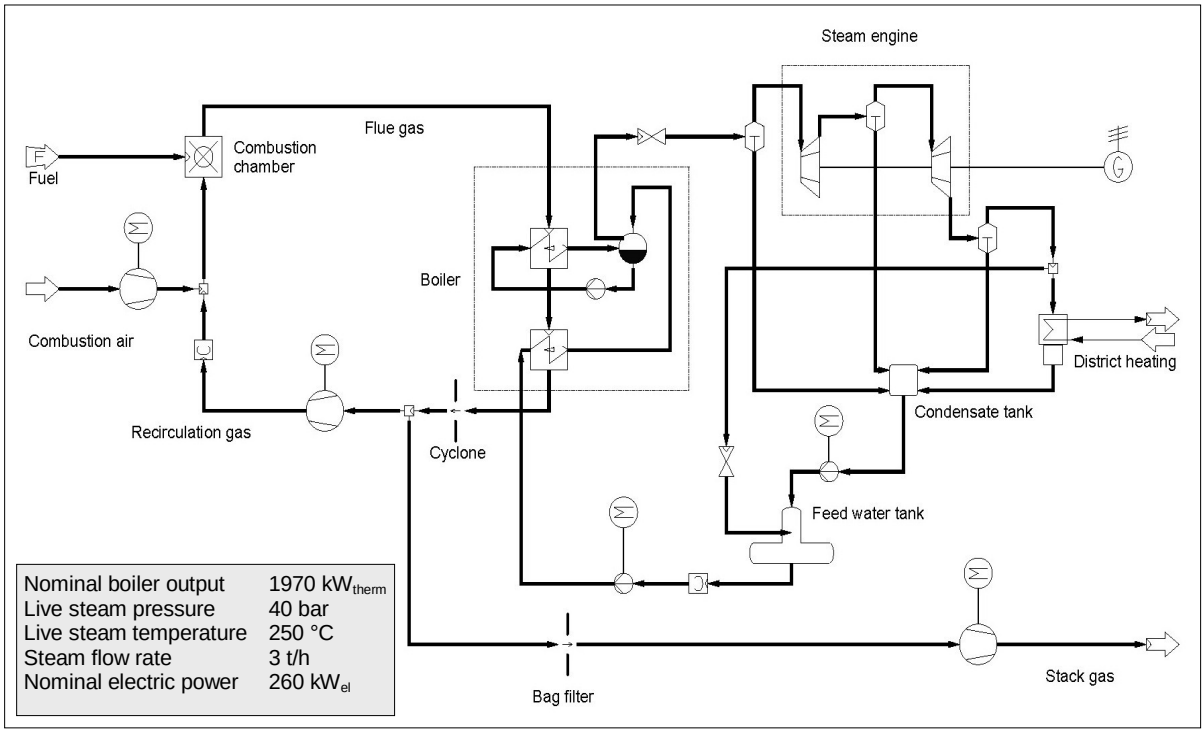
In the recent years, a software tool for improvement of the basic engineering of fluegas cleaning processes has been developed together with the Austrian Energy & Environment AG (AE&E). By means of steady-state flowsheet simulation, the basic key figures of a fluegas cleaning plant can be predicted and the optimum design in ecological as well as economical respect can be found. 2004, a joint study on three different plant setups for emission control after incineration of domestic waste has been conducted. The following figure shows a comparison of the fractioned operating costs for meeting the legal emission limits (17. BimSchV) at an exemplary Austrian location. Obviously, solid waste and the corresponding costs of disposal are governing the balance:



Legend: Fractioned operating costs of three different processes for fluegas cleaning (Dry … dry process/no water usage, Wet … wet process/no waste water, Wet WW … wet process/waste water), HM … Heavy Metals

PROCESSSIMULATION OF A BALED BIOMASS FIRED CHP PILOT PLANT

The simulation of a CHP cycle connected to a combustion plant for baled biomass with an output of $2MW_{thermal}$ has been carried out in cooperation with Greenpower and was subsidized by the EU. The flow sheet of the pilot plant is shown below.



Flow sheet of the biomass fired CHP pilot plant in IPSEpro®

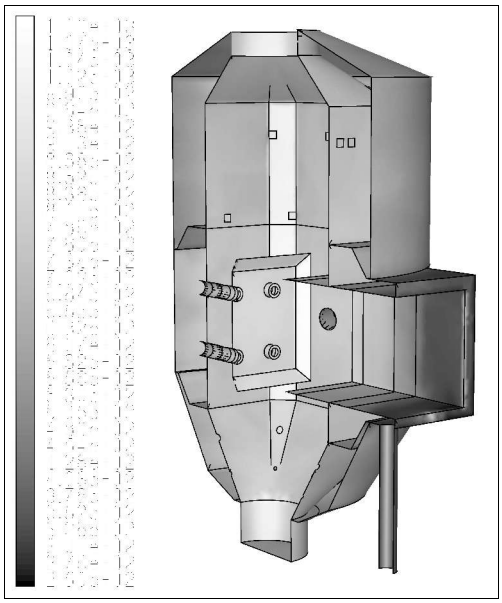
After the buildup of a flow sheet that represented the pilot plant correctly, variations of the air ratio, the stack gas temperature and the live steam pressure were carried out in order to maximize the electrical efficiency of the pilot plant. Furthermore steam cycles with additional exhaust steam turbines and variations of the boiler have been simulated to find a steam cycle layout that is most suitable for small and medium biomass plants. The further work of the project includes the scale up of the plant and the optimization of the parameters and the layout.

2.2 COMPUTATIONAL FLUID DYNAMICS & THERMAL PROCESS ENGINEERING

Information about further CFD research activities is available on our CFD activities homepage http://www.cfd.at, information about membrane related group activities can be found here: http://www.membran.at.

CFD- SIMULATION FOR A BALED BIOMASS COMBUSTION SYSTEM

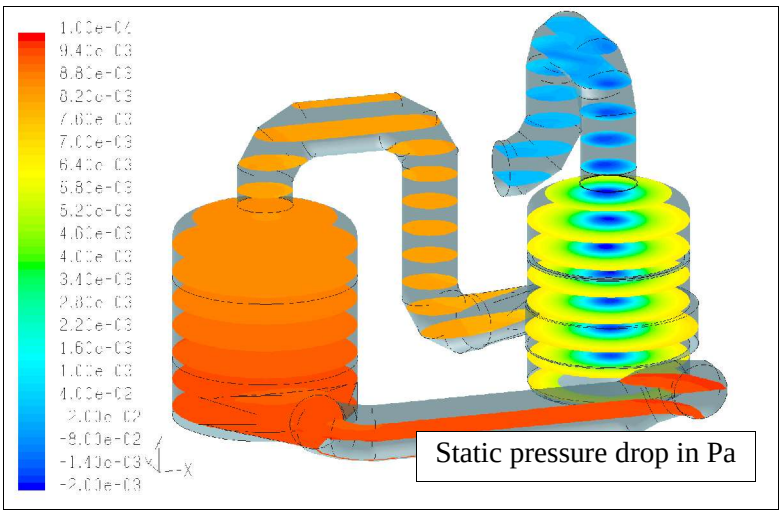
The commissioning and optimization of an innovative combustion chamber for baled biomass has been supported by the accomplishment of fluid dynamic simulations. This project is conducted in cooperation with Greenpower and Herz and is subsidized by the EU. Due to the complexity of this new combustion concept numerous advanced calculation models had to be applied to assure correct simulation results. These models concern the description of



turbulence, radiation, homogeneous and heterogeneous biomass gasification and combustion and fly ash burnout. The selection and parameterization of these calculation models has been assisted by experimental results gathered at a combustion pilot plant with 2MW thermal output. The results of the flow simulations are used for design improvements to enhance the thermal efficiency as well as the operating behavior and to reduce the emissions of carbon monoxide, nitrogen oxide and dust. To depict one of these results exemplarily the calculated combustion chamber wall temperatures are shown in the picture. This analysis is helpful for choosing the proper steel grade for the shell as well as for the identification of "hot spots" inside the combustion chamber where danger of slagging and high temperature corrosion can be expected. All calculations were performed using the commercial CFD-solver FLUENT 6 on a multi-processor cluster-platform.

CFD-SIMULATION OF A CYCLONIC DEMISTER

Cyclonic Separators are not only used for particle separation, they are also successfully employed in demisting and droplet separation. In this study a demister is simulated which is operated in forward flow direction (in contrary to the typical reverse flow type cyclones). Despite this unusual geometry the resulting flow features and the pressure drop are similar to the standard type.



Static pressure drop in Pa

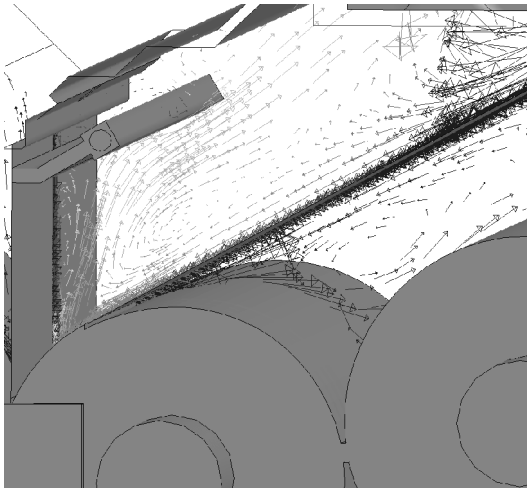
Geometry implementation was done using the pre-processor GAMBIT (Fluent Inc., further information is available at http://www.fluent.com). The flow field calculations have been performed with the commercial CFD code FLUENT (also Fluent Inc.) which is based on the finite volume approach. Again it was necessary to use the Reynolds stress turbulence model to capture the anisotropic shear stress distribution in the strongly swirling flow.
In cooperation with Vogelbusch GmbH a strategy for the reduction of the pressure drop for this type of demister was evaluated and an optimized configuration of the guide vanes was determined. Further investigations concerning the impact of other geometrical parameters on the pressure drop are in progress.

CFD-SIMULATION OF AIR FLOW IN A PAPER LAMINATING MACHINE

Computational Fluid Dynamics (CFD) is a powerful tool for analysing and optimizing complex flows for industrial applications. The partner in this project was SIG Combibloc GmbH, a Swiss based company and global provider of packaging materials and equipment for bottling of beverages.

The goal of the collaboration was the design of a novel ventilation for fumes and gases produced in the laminating process ensuring compliance to threshold limit values without compromising product quality at the same time.

Implementing the complex geometry was a great challenge and yielded over 1600 separate volumes containing 1,6 million finite volume cells. Most important was the correct discretization and simulation of the boundary flow introduced by the fast moving paper (> 8 m/s) and cylinders which is the main cause of emission and dilution. A "worst case scenario" was assumed for simulation parameters to be on the safe side with results. Several geometry variations depending on production conditions were simulated. Finally, a ventilation based on analysis of CFD-results was constructed which effectively reduced the emission by more than 70% compared to the original setup without product quality losses.

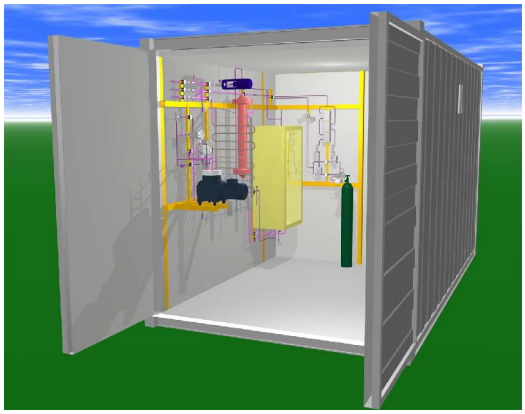


Geometry detail and velocity vectors

EFFICIENT UPGRADING OF BIOGAS USING MEMBRANE SEPARATION PROCESSES

Biogas produced from grass or energy crops is a gas mixture containing methane (55-75%), carbon dioxide (23-43%), hydrogen (< 2%) and traces of hydrogen sulphide and ammonia. Biogas when produced is saturated with water. Biogas can be used for several purposes: direct combustion, combined heat and power generation, compression and usage as fuel, and the usage as a natural gas substitute after upgrading and compression. For the usage as a natural gas substitute it is important to develop an efficient and robust technology to remove carbon dioxide, humidity and the traces of ammonia and hydrogen sulphide for the specific requirements in rural areas where current technologies have certain disadvantages.

It is the main goal of this project funded by FFG (Project Call "Energy Systems of the Future", Project 807739, http://www.edz.at, see also http://www.membran.at) to develop a modern efficient method based on a membrane separation technology and to test the technology in combination with a biogas fermentation for the digestion of energy crops. Another goal of the project involves the screening of new gas analysis techniques for the online monitoring of the product gas in collaboration with the Institute of Chemical Technology and Analytics. Safety measures for the scale up of the technology and suitable control techniques will be investigated and recommendations will be given. Additionally, a simulation tool is being developed to model and scale up the investigated technology.



Container design study

2.3 CHEMOMETRICS

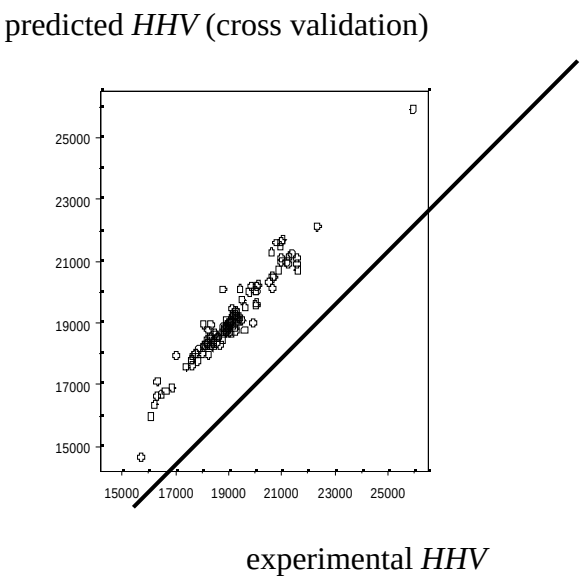
Homepage of the Laboratory for Chemometrics (LCM): http://www.lcm.tuwien.ac.at

PREDICTION OF HEATING VALUES OF BIOMASS FUEL FROM ELEMENTAL COMPOSITION

The heating value of biomass is an important parameter for the design and the control of power plants using this type of fuel. The so called higher heating value, *HHV*, is the enthalpy of complete combustion of a fuel including the condensation enthalpy of formed water. Numerous empirical equations have been published to relate the heating value of fuel to the elemental composition of fuel as obtained by elemental analysis. Early mathematical models that relate the heating value to the amount of carbon, hydrogen, nitrogen, oxygen, and sulfur date back to the late 19th century. Many models have been suggested for coal; recently models for municipal solid waste have been derived, but only a few attempts consider biomass fuel.

Data of 154 biomass samples of very different origin (for instance wood, grass, rye, rape, reed, brewery waste, and poultry litter) have been selected from the database BIOBIB. Each sample has been characterized by the contents (in mass % of dry material) of carbon, hydrogen, nitrogen, oxygen, sulfur, chlorine, and ash. Principal component analysis of these data shows a clustering according to the origin of the samples.

A subset of 122 samples, all consisting of plant materials, has been used to develop regression models for a prediction of *HHV* from the elemental composition. Models with best predictive ability have been obtained using the contents of carbon, *C*, hydrogen, *H*, and nitrogen, *N*, and applying PLS regression with the variables *C*, C^2, *H*, *C.H*, and *N*. The standard errors of prediction of the best new models are considerably smaller than those obtained with models found in literature.



Predicted versus experimental *HHV* [kJ/kg] for plant biomass. A leave-one-out cross validation (CV) has been applied with PLS linear regression. Measurements used are mass% of carbon, hydrogen, and nitrogen in dry biomass. Standard error of prediction (equivalent to standard deviation of prediction errors), SEP_{CV}, is 372 kJ/kg; squared correlation coefficient, R_{CV}^2, is 0.935.

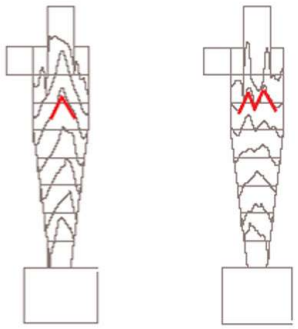
A. Friedl, E. Padouvas, H. Rotter, K. Varmuza: Anal. Chim. Acta, in print (2005)

http://www.lcm.tuwien.ac.at/vk/Manus/Lisbon-CAC2004-biomass-poster.pdf

The new equation for prediction of the higher heating value of plant biomass may be of practical interest in power plant construction in the stage of basic and detail engineering of plants that use biomass fuels alone or even mixtures with other fuels. Also plausibility checks of experimentally determined heating values can be performed with the new equation.

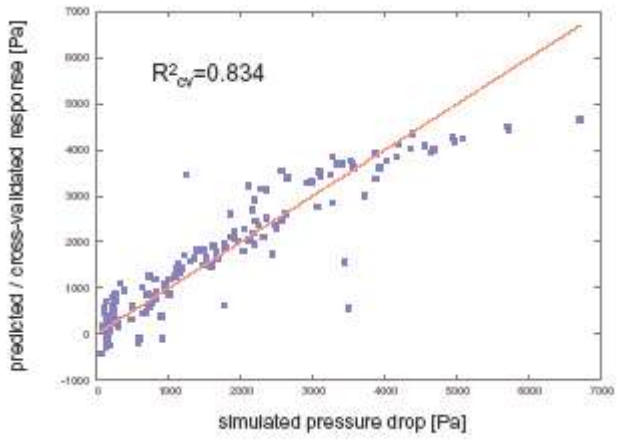
COMPUTATIONAL FLUID DYNAMICS SIMULATION COMBINED WITH CHEMOMETRIC METHODS

Several types of flow structures in cyclones were reported in recent publications. The flow structures were split into two classes, each representing a certain type of axial velocity profile of the gas flow inside the cyclone. Class “V” are cyclones with a maximum of the axial velocity at the vortex core of the cyclone, whereas class “W” represents cyclones with an axial velocity profile that resembles an upside down character “W”. This class has a local minimum of axial velocity at the vortex core or even displays backflow. The geometries belonging either to class “V” or class “W” showed only small relative differences.



The figures show examples of profiles "V" and "W" of axial velocity of geometrically similar cyclones (constant volumetric flow rate). Results have been obtained by computational fluid dynamics (CFD) simulations. To determine the influence of various geometric parameters on the internal flow structure and thus on the class membership, 144 computational fluid dynamics (CFD) simulations were carried out.

The obtained simulation results (one simulation requires about 24 hours computation time) have been used for multivariate classification of the flow profile class, and to model the pressure drop from geometrical parameters. Such models have the advantage to produce results very fast, however, have some error rate. K-nearest neighbor classification yielded 85% correct assignments to class "V" and "W" (leave-one-out cross validation).



Linear PLS regression allows a fast semi-quantitative prediction of the pressure drop from geometric parameters of the cyclon and the inlet velocity.

A. Horvath, C. Jordan, M. Harasek, K. Varmuza:
http://www.lcm.tuwien.ac.at/vk/Manus/Balaton-SCAC2004-cyclone-poster.pdf

The application of chemometric methods for postprocessing of CFD results is a promising new approach to classify flow behavior of complex gas flows and to find geometry – flow relationships. Applications are not limited to chemical engineering problems.