# Annual report 2011


E4-Mistra is a research programme that develops an energy efficient low emission aftertreatment system.

## Contents



E4-Mistra is a joint research initiative between academic and industrial partners:

Chalmers University of Technology
Royal Institute of Technology

Höganäs AB
Termo-Gen AB
Volvo Technology AB
Alfa Laval AB

E4-Mistra, Annual report, 2011
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# From the chairman

It seems probable that activities of mankind, while developing our civilisation, are threatening the biosphere in which we live. Our wish to improve our living standard has meant increased energy consumption and pollution. Up till recently focus has been on recreating clean air, clean water and clean soil. But now it seems we must to come to rescue of the earth's climate as a whole.

To combat the problems we have to make full use of our capacity for technological development. But this will not be enough. We also need to organise this work in an efficient, industrial way and utilise the same driving forces in the preservation of the climate that previously have given mankind improvements in many other areas.

E4 is a programme composed in that way. It is hosted by Volvo, engages other competent industrial companies, and mobilises academic competencies at the highest level. The goal is to reduce the emissions from transportation with diesel engines while at the same time reducing energy consumption. The programme involves a couple of innovative approaches, thermoelectric materials, efficient catalysers utilising reformed fuel and improved filter types. Combination of these innovative measures with the business capacity from the companies involved should allow a substantial contribution to the efforts to preserve our environment and climate.

*Thomas Johannesson*

# Background

Emissions of particulates and nitrogen oxides from new heavy duty vehicles have decreased significantly during the last decade. Within the next five years, the exhaust emissions from heavy duty diesel engines in Europe, the US and Japan will reach levels that may be accepted as sustainable for the long term.

Commercial vehicle manufacturers have always strived for lowering fuel consumption, but the focus has become even stronger as both fuel costs and environmental concerns have increased among the users of the vehicles. New legislation regarding carbon dioxide emissions will also soon be in place in many countries, and this will create demands for engines and vehicles that consume less fuel. The new legislation will also create incitements for technology that may be too costly to pay for itself on short-term basis, but, required in order to fulfil the carbon dioxide emission limits.

The consumption of fuel used for commercial transportation may be reduced by several methods. The transport efficiency may be increased by allowing longer or heavier vehicles or by improving the transport logistics. The vehicle's fuel consumption may decrease by lowering the air drag or rolling resistance or by incorporating hybrid technology. The impact of these improvements is typically larger than the improvements that may be achieved in the diesel engine.

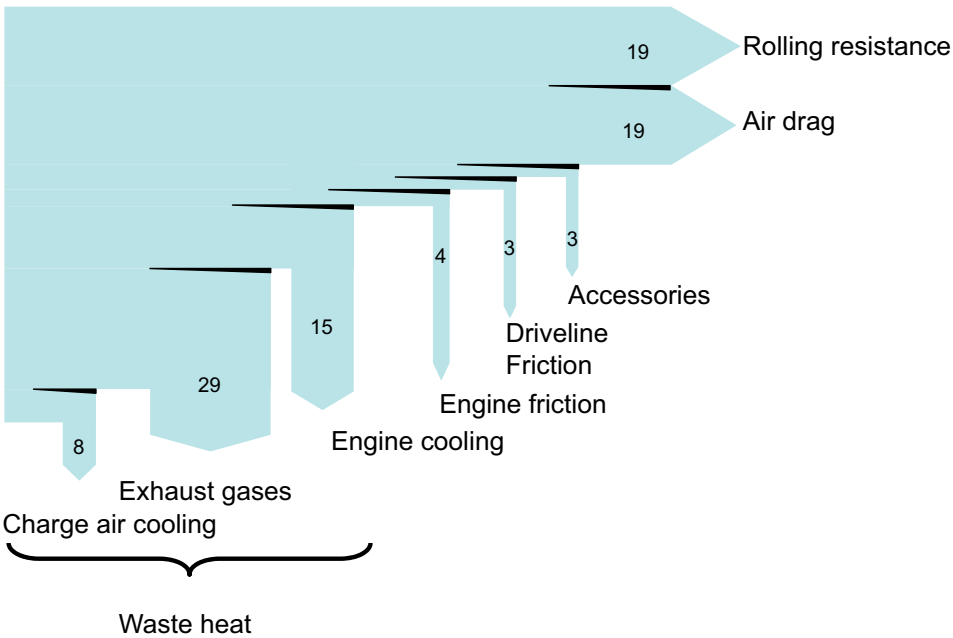
A typical energy distribution for a long-haul truck is shown in the figure. Less than 40 % of the energy in the diesel fuel is used for actual work, and more than 50 % is lost as heat, either in the exhaust gases or in the cooling system. Recovering part of the energy that is lost in the exhaust gases and using this energy for propelling the vehicle can have a large impact on the overall fuel consumption.

The energy in the exhaust line may be recovered by expanding the exhaust in a second turbine, a turbo compound system. The work developed in the second turbine is either mechanically or electrically transferred to the driveline. The warm exhaust gases may also transfer heat through a heat exchanger to a Rankine engine. A steam engine is a Rankine cycle based on water as the working fluid, but other working media may also be used.

A third option is to use a thermoelectric device for recovering heat from the exhausts. A temperature difference in a heat exchanger is directly converted to an electric current, and the electric power may be used for charging the batteries in a conventional or hybrid drive train.

All efforts to use the energy in the exhaust must be balanced by the requirements of the exhaust aftertreatment system. The exhaust temperature for many common types of commercial vehicles are close to the lower limits where the catalyst are active, and a careful integration of waste heat recovery technologies is therefore required to improve the catalytic activity.

The demands for reducing $NO_x$ and particles emissions to meet the legislation targets, in additions to the need for improved overall system efficiency and optimized utilization of available energy for enhanced system performance are the major driving forces for the initiation of this ongoing E4 Mistra programme which is now in its second phase. During the first phase which was running between 2006-2010, promising results within fuel reforming, $NO_x$ reduction activities and waste heat recuperation by thermoelectric generators were achieved. The focus of the second phase (2010-2014) is to further improve the applied technologies, secure the functionality and stability of the integrated system, and utilize suitable renewable fuels as alternatives to fossil fuel to decrease the emission of fossil $CO_2$.

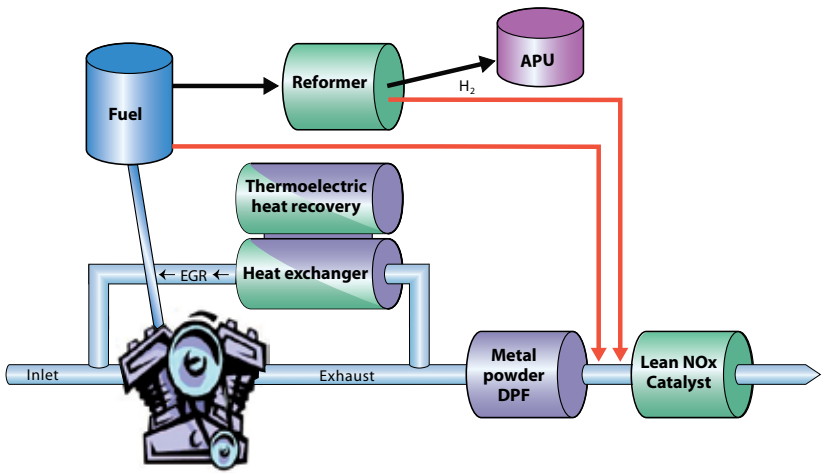



Schematic illustration of energy distribution for a long-haul truck running at 90 km/h on flat road.

# The programme

A unique system approach is applied in this programme to reach the goals of energy efficiency and low emissions. The high energy efficiency is achieved by heat recuperation, on-board hydrogen production for use in both an auxiliary power unit and for $NO_x$ reduction and by finding new solutions for making the after-treatment system active at low exhaust temperatures. To reach low particulate emissions a mechanical filter using a sintered metal filter is developed. Low $NO_x$ emissions are achieved by an efficient $NO_x$ reduction catalyst.

The system is based on four technological advances: Thermoelectric materials for heat recuperation, catalytic reduction of $NO_x$ over innovative catalyst substrates using hydrocarbons from the fuel and $H_2$ from a high efficiency fuel reformer, and particulate filtration over a porous metal filter. The figure illustrates how the individual components can be connected in an integrated system




Relation between the different components in the programme.

The programme is organized in eight component projects. Each component project is important for the integrated result. To achieve smooth interfaces between the components, the projects participants meet frequently to discuss the entire system. In this way, the programme represents an interdisciplinary approach to advance present technology. This report briefly describes the progress during 2011.

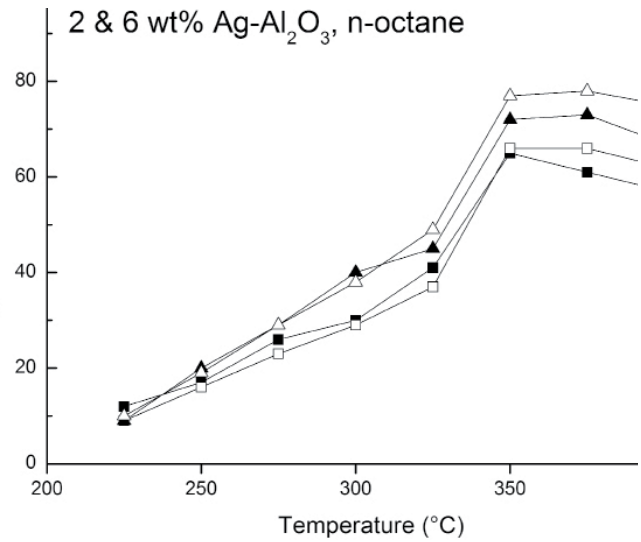
## Catalytic reduction of $NO_X$

Hanna Härelind Ingelsten

Although new propulsion systems are emerging, combustion systems with excess oxygen, like diesel- and lean-burn engines, will likely continue to be important engine systems during the next few decades. Particularly interesting is the possibility to run these engines on alternative fuels and thereby lowering the emissions of fossil $CO_2$. One important draw-back with lean combustion is, however, the formation of nitrogen oxides ($NO_x$). In order to convert $NO_x$ to $N_2$ in oxygen excess, development of new catalyst concepts are required. Within this component project a catalyst will be developed for energy efficient reduction of $NO_x$. The research will focus on new, innovative catalyst concepts for continuous reduction using hydrocarbons from the fuel (with focus on renewable fuels) and/or hydrogen from the reformer as reducing agents.

During 2010 Fisher-Tropsch diesel, bio-diesel (based on FAME) and methanol were identified as alternative fuels to be included during the course of the programme. Since the catalytic activity for lean $NO_x$ reduction is strongly dependent on the type of reducing agent, design, preparation and evaluation of new catalytic materials for some of the alternative fuels mentioned above has been the focus during this year. Furthermore, the performance of aged catalysts with different reducing agents has been investigated.

This year syntheses of improved catalytic samples have been performed using the sol-gel method, which was developed during the first phase of this component project. The catalyst samples have been thoroughly characterized concerning *e.g.* surface area and composition, silver phase and particle size, and catalytic activity for $NO_x$ reduction. In particular $NO_x$ reduction activity experiments with simulated exhaust gases where the catalytic performance with different reducing agents, *i.e.* bio-diesel, diesel from fossil oil and n-octane, has been compared. Some of our samples have also been evaluated for catalytic activity in the synthetic gas bench at Volvo using the same type of reducing agents. During the year we have also continued the ageing study, and in particular compared the ageing performance for several improved catalyst formulations with bio-diesel and n-octane as reducing agents (as illustrated in the figure).




$NO_x$ conversion as a function of temperature over various silver-alumina catalysts, using bio-diesel (NExBTL) as reducing agent.

The component project, catalytic reduction of $NO_x$, has during 2011 been performed by Fredrik Gunnarsson and Hanna Härelind Ingelsten at the Competence Centre for Catalysis, Chalmers University of Technology.

Anders Palmqvist

## Thermoelectric materials

During 2011, the PhD student Yi Ma graduated with a thesis on electrochemical deposition and characterization of thermoelectric thin films of bismuth telluride and its derivatives. Yi Ma continues as a one-year postdoc in the E4 Mistra programme during 2012 exploring bulk thermoelectric materials of more sustainable elemental compositions. The second PhD student in this project, Daniel Cederkrantz has defended his PhD thesis in February 2012. The third PhD student Richard Heijl has gained momentum and is now carrying the main part of the component project forward in this the second phase.

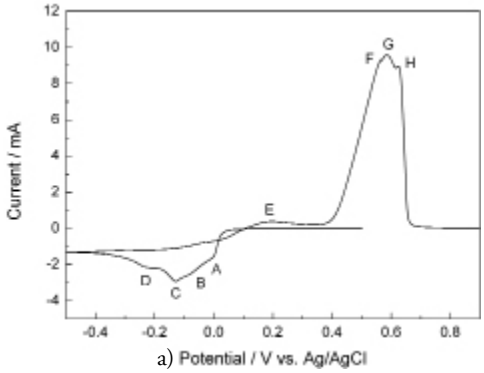
The aim of this component project is to develop more efficient thermoelectric materials for use in the thermoelectric generator to be prepared by TermoGen. Such generators convert thermal gradients into electricity and require two types of thermoelectric materials for their function, a p-type and an n-type semiconductor, connected electrically in series and thermally in parallel.

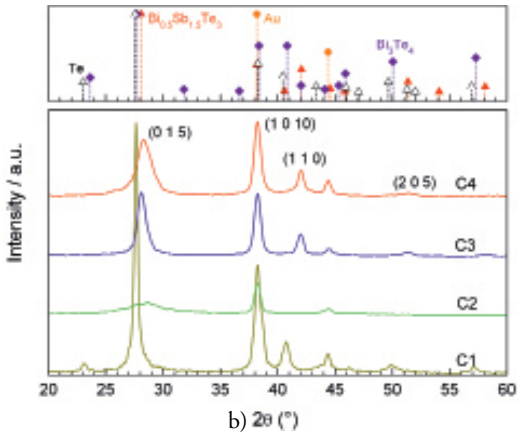
A high performing component thermoelectric material has a high figure of merit, $ZT = S^2\sigma T/\kappa$, at the desired temperature T, where S is the Seebeck coefficient, $\sigma$ is the electrical conductivity and $\kappa$ is the thermal conductivity, all of which are temperature-dependent. Thermal conductivity consists of lattice vibrations and heat-conduction through electronic conduction, which means that to improve ZT one may target to preferably lower the lattice vibration part of $\kappa$ to avoid lowering $\sigma$ as much.

We continue to follow two different concepts towards new efficient thermoelectric materials. The first is the phonon-glass-electron-crystal (PGEC) concept in which host guest structures are used to efficiently reduce the lattice vibration part of the thermal conductivity of the material without losing too much in electronic conduction. In the second concept we seek to exploit some of the positive effects that nanostructuring may have on thermoelectric materials performance.

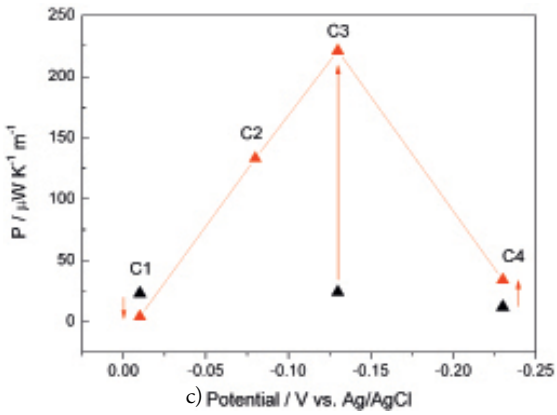
Our focus along the PGEC route during 2011 was on inorganic clathrates, where we have evaluated the effects of introducing nanoinclusions of a heterocompound in the matrix of the clathrate, and prepared a manuscript for submission. An exploratory study of similar character performed on the more environmentally benign magnesium silicide system has been published and we are following this up with another study during 2012.

Targeting the colder side of the thermoelectric generator (below 250°C), development of suitable processing conditions for electrochemical deposition of nanostructured $Bi_2Te_3$ and $Sb_2Te_3$ films and their derivatives of relevance for multilayer deposition has been carried out and resulted in three accepted publications in 2011 and early 2012.




a) Cyclic voltammogram of a 1 M HNO3 solution containing 10.0 mM $HTeO_2^+$, 1.5 mM $Bi^{3+}$, 3.0 mM $[Sb_2(C_4H_4O_6)_2]^{2+}$, and 0.67 M tartaric acid starting at open circuit potential and with a sweep rate of 10 $mVs^{-1}$ on Au-coated Si substrate. b) XRD patterns of four thin films formed by electrodeposition using slightly different potentials around peak C in a) showing formation of targeted $Bi_{0.5}Sb_{1.5}Te_3$ under suitable conditions. c) Power factors of films prepared in b) showing importance of deposition conditions and improvement by annealing films (red) under inert conditions at 130°C.

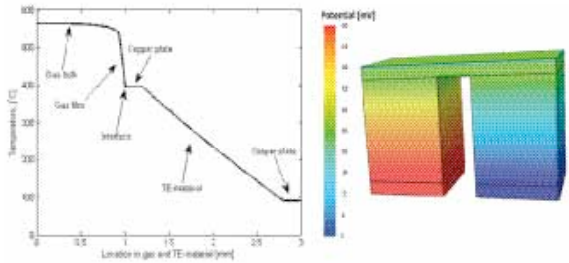



This component project is performed by Daniel Cedercrantz, Yi Ma, Richard Heijl and Anders Palmqvist, at Applied Surface Chemistry, Chalmers University of Technology.

Ronnie Andersson

## CFD for heat exchangers

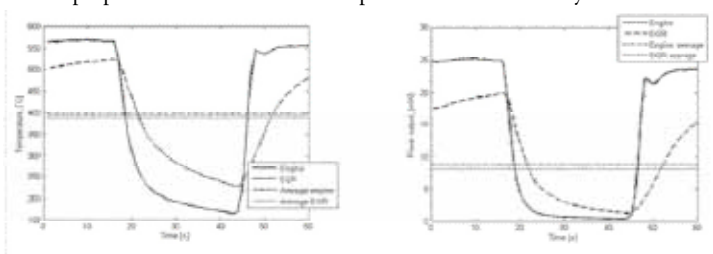
The progress made during 2011 includes among others the development of a new in-house code, UDF (user defined functions), for the CFD simulations. Besides the prediction of heat transfer and power generation, these simulations give detailed insight to the temperature gradients in the gas-phase and inside the solid TE elements. One conclusion from this study is that a large heat transfer resistance occurs on the exhaust gas side, as shown in the first figure. This reduces the overall efficiency of the TEG systems, and the temperature drop on the gas side must significantly be reduced to increase the TE material surface temperature.



Temperature distribution in the TEG-EGR system and contour plot of the total potential in a thermocouple.

One possible solution to reduce the heat transfer resistance was identified during one TEG design workshop. CFD simulations at Chalmers and prototype tests at Alfa Laval recently confirmed improved performance using this new design with respect to heat transfer and pressure drop. During 2011 we also did simulations of TE-elements coupled in series.

TEG performance simulations during a reduced vehicle cycle were presented at the 9th European Conference on Thermoelectrics. The paper "Högblom, O., Andersson, R., *CFD Modeling of Thermoelectric Generators in Automotive EGR-coolers*" summarizes the findings. The temperature and transient power generation during a reduced vehicle cycle is shown in the second figure. In this study the thermoelectric properties of the material developed at Surface Chemistry was used.



Combustion and EGR temperatures.

Transient power generation.

Besides these activities the CFD team participated in new TEG design workshops during 2011 and in August 2011 we also organized a PhD course 'Introduction to CFD' at Chalmers, within the frame of the E4 MISTRA programme.

During 2012 we plan to do validation using upcoming TEG prototype test results at Alfa Laval and Volvo. The prototype will be studied at different flow rates, flow configurations, temperatures and electrical load. Further analysis of improved heat transfer designs, discussed within the TEG group, also needs to be done to establish design guidelines. In addition to this simulation of the TEG prototype from Termo-Gen AB is planned.

This component project is performed by Olle Högblom, Ronnie Andersson and Bengt Andersson, Chemical Reaction Engineering, Chalmers University of Technology.

## Reformers for hydrogen production

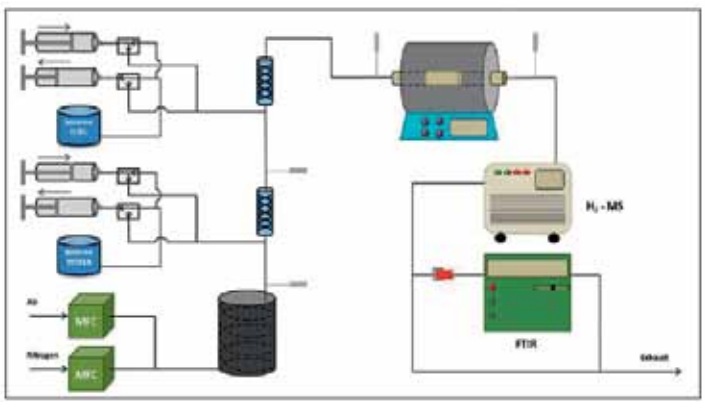
Lars J Pettersson

This component project focuses on hydrogen generation from conventional motor fuels as well as fuels produced from renewable feedstocks. Hydrogen can be used at oil refineries to produce more environmentally-friendly motor fuels by decreasing the sulphur and aromatics content of diesel fuel using hydrodesulfurization and hydrodearomatization. The E4 Mistra programme is focused on heavy-duty trucks where hydrogen can be used in an auxiliary power unit supplying electricity at stand still or for increasing the activity of de$NO_x$ catalysts. The latter method has been studied in close collaboration with Chalmers while using their silver/alumina catalyst. The results from this study were published in Applied Catalysis B: Environmental during the year.

One of the highlights of 2011 was that Xanthias Karatzas successfully defended his PhD thesis "Rhodium diesel-reforming catalyst for fuel cell applications" on April 29 at KTH. The faculty opponent was Professor James Spivey from the chemical engineering department of Louisiana State University in Baton Rouge, USA. One of the important outcomes of the thesis is that we have obtained a better understanding of diesel reforming catalysts. Interesting findings are how various materials interact on the surface and how this affects the activity and selectivity of the catalyst.

The price of precious metals has increased during the last years due to the instability of world economy. In this phase we are investigating the possibility to reduce the precious metal content of the rhodium-based catalyst by adding various metal oxides. The first experimental series performed in the laboratories of Volvo Technology resulted in promising results regarding activity and hydrogen selectivity. However, the stability of the catalysts needs to be improved.

We have designed and constructed a test rig for evaluation of the performance of catalysts for autothermal reforming of hydrocarbon fuels in both liquid and gaseous state (see figure below). With some modifications we can also test other advanced small-scale reactor designs, such as microreactors. The test rig is prepared for change of reactor and diesel evaporator. The product gas is analyzed using on-line continuous instruments. A mass spectrometer is used to analyze hydrogen and the other compounds are detected by using FTIR and gas chromatography.




Miniature catalyst activity evaluation test rig. MFC: Mass Flow Controller; MS: Mass Spectrometer; FTIR: Fourier Transform Infra-Red Spectrometer.

This component project is performed by Moa Ziethén Granlund, Xanthias Karatzas and Lars J. Pettersson at Chemical Engineering and Technology, KTH Royal Institute of Technology.

Lennart Holmgren

## Thermoelectric devices for power generation

The objective for this component project is to develop a Thermoelectric generator (TEG) based on thermoelectric materials developed at Applied Surface Chemistry, Chalmers University of Technology. The TEG heat exchanger system is developed in cooperation with Chalmers and Alfa Laval. The test of the TEG is done in-house and at the engine laboratories at Volvo.

The TEG will be used for recuperation of heat from the EGR circuit of heavy trucks. The available heat power is up to 30kW and the TEG power is expected to reach 2 kW. The electric power from the TEG is intended to increase the total energy efficiency of the vehicle and the after-treatment system developed in the project.

The work in 2012 has been focused on the development of an integrated TEG-heat exchanger (TEG-HEX) in close cooperation with Volvo, TYK, Alfa Laval and KRT. We have delivered test modules for the test Alfa Laval set-up and contributed with our previous experience.

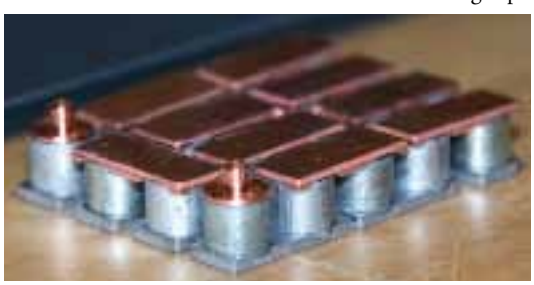
A second objective has been to work on the module design and test where we are developing flat high temperature modules for operating at a hot side temperature of 600°C. The flat modules are based on the technology of our cylindrical modules. A successful 3500 h test has been done on a 16 W cylindrical mini-module at a hot side temperature of 550°C and a 6300 h test on a flat six-couple test module. The degradation rate is linear and approximately 2 W per 2000 h for the 16 W module. It is a good result but we are now working to reduce the degradation rate further.

Three 1000 h long term tests have been done for three versions of the lower temperature Bi2Te3 modules. The modules were operating at a hot side temperature of 250°C with stable performance. A short term test at 350°C showed a rapid degradation within 10 hours for the first version. A new method for stabilising the modules for use at operating temperatures up to 380°C has been implemented on the modules in the ongoing test.

The work on the first prototype based on heat pipes and flat Bi2Te3 modules has continued. The engine bench run has been delayed until Q2 2012. The TEG has been modified with a new module set-up with lower heat conductivity adjusted to the actual heat flow in the application. The first verification will be performed at Termo-Gen and the engine bench tests will be done at Volvo.

Work has been done on improving the powder compaction of thermoelectric elements for the TEG modules. Fine grained powder has to be granulated to be used in the high speed press to avoid dust and reduce downtime. We are presently making a test series with freeze granulation of different TEG materials grinded in the Pulverisette premium line 7 planetary mill to sub-micron powder size. The objective is to make compacts of equal or better quality compared to compacts made by the present method. The clathrate powder produced by TYK will also be freeze granulated.

We are developing suitable process parameters for the compaction and after-treatment of the freeze granulated powders for each material family in the project.



3 W PbTe module, 25 x 31 mm

This component project is performed by Lennart Holmgren, Gerd Holmgren and Vivianne Svensson at Termo-Gen AB.

## Heat exchanger for thermoelectric generators

The "heat exchangers for thermoelectric generators" project aims at developing a feasible interface between plate-based heat exchangers and thermoelectric generators.

As a result from a workshop held at Alfa Laval in 2010 we have during 2011 been working on developing and manufacturing a demonstrator to, in a flexible way, study the thermoelectric generator in combination with our own plate based heat exchanger technology.

The demonstrator was designed so that it would be representative for a possible future solution based on our materials, technology and process. However, during the manufacturing and assembly we learned more about the conditions required for the thermoelectric generators and had to make changes that made it less representative.

The demonstrator has at the end of 2011 been tested in our laboratory facility with high temperature gas to allow us to gather and build knowledge on the feasibility of the combination of technologies.

During the development of the demonstrator we have identified several major challenges that our technology creates for the conditions that is required for the thermoelectric generator to function efficiently and durable.

Furthermore, we have continued our studies on the high temperature properties of our plate-based heat exchanger technology and the possibilities to improve for high volume manufacturing of these materials.

Fredrik Andreasson

Equipment for study of heat transfer to thermoelectric module at Alfa Laval.

This component project is performed by Magnus Svensson, Fredrik Strömer and Fredrik Andreasson at Alfa Laval.

Per-Olof Larsson

## Metal powder filter

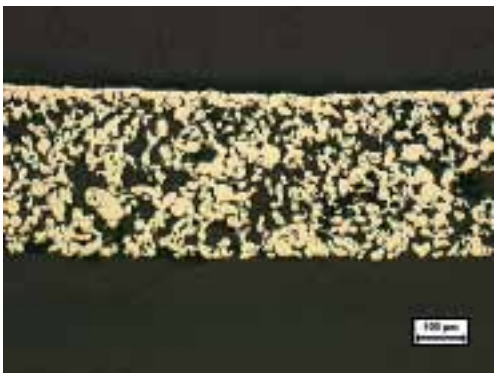
Höganäs AB has delivered metal powder based diesel particulate filters, based on designs developed together with Volvo Technology, to the project. For the last prototype, Höganäs has developed a method to sinter porous filter sheets and corrugated solid sheets together into one stack. In addition, Höganäs has developed a metal powder paste for sealing, which can be applied on the edges and sintered. This has resulted in a delivery of a sintered complete filter stack that is sealed between the porous filter sheets and the corrugated sheets as well as at the edges. The filter stack has been tested as a 1.8 litre DPF in the one-cylinder rig at Volvo Technology. Good results at steady state operation with filtration efficiencies around 99.5% were obtained, even at very high pressure drops, which show that the sealing problems in the beginning of the project can be avoided. Activities are now ongoing in order to verify the increased ash storage capacity of the filter design in accelerated tests at Volvo Technology.

Höganäs has evaluated extrusion as a technology for production of porous metal powder structures. The objective with the extrusion has been to identify production pathways that do not include corrugated sheets, and make fabrication of stacks consisting only of metal powder possible. Höganäs has developed different water based extrusion pastes containing metal powders. Using different tools it has so far been found that it is possible to make tubular shapes with wall thicknesses down to approximately 600 µm when the diameter is 6 mm, but most likely it is possible to make thinner tubes if the diameter is reduced further. However, extrusion is not possible for the sheets used in the DPF design in the project today. These are too thin (400 µm) and too large (200 mm in width). If extrusion should be used, the design of the present DPF prototype would have to be changed.

Höganäs has been working with material development in order to improve the performance and lower the cost for the metal powder. The focus in the beginning of the project was to decrease the cost by lowering or removing the nickel content in stainless steel 310B (25% Cr, 20% Ni, 2.5% Si, Bal. Fe), and by optimizing the particle size distribution. With time it also became clear that it would be desirable to coat the DPF with catalytic materials. This means that a washcoat with catalytic material should be attached to the stainless steel surface. In order to improve the adherence between the stainless steel and the applied washcoat, it is probably required that the thermal expansion coefficients (TEC) of the both materials are similar. Since the TEC for ferritic stainless steels is closer to the TEC for ceramic materials than the TEC found for austenitic stainless steels, it could be an advantage to have a ferritic stainless steel material in coated diesel particulate filters. Höganäs has found that different ferritic stainless steel materials based on Fe with 20-22% Cr have more and less the same high temperature oxidation resistance as 310B, while the TEC matches the ceramic materials better, and a lower raw material cost is possible due to the absence of Ni.

In addition, theoretical as well as experimental activities have been started for the development of procedures for washcoating of the porous metal power sheets. Washcoat experiments have thus already been made on both ferritic and austenitic stainless steels. The first challenge has been to obtain a uniform washcoat layer at macro scale on porous metal sheets.

More dense surface layers on the porous sheets may be advantageous in order to reduce deep filtration. This could perhaps also improve the ash storage capacity further for the proposed design. Höganäs has developed two different methods to obtain a gradient porosity structure in the sintered metal powder sheets.



Light optical microcopy picture of a cross section of a sintered metal powder sheet with a gradient porosity structure.

This component project is performed by Per-Olof Larsson, Jörgen Knuth-Nielsen and Ivan Smirnov at Höganäs AB.

Jazaer Dawody

## System integration and validation

Although the different E4 Mistra system components are developed and tested within the corresponding component projects, it is essential to evaluate the performance of the individual components as well as the integrated system under realistic conditions, *i.e.* in this case, diesel engine exhaust gas conditions which is one important target for the system validation and integration project component. Another important target for this project component is to support the development of the individual components by providing system boundary conditions including relevant exhaust gas data and reporting on the state of the art technologies for exhaust aftertreatment system components and performance of existing systems.

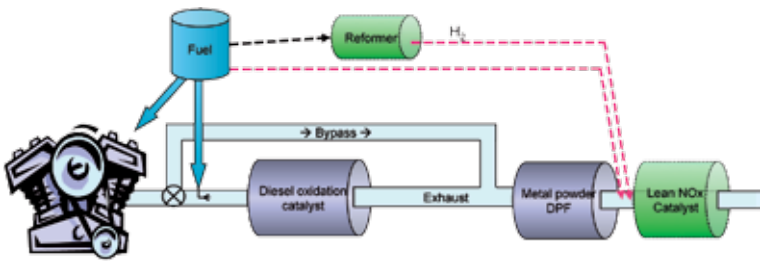
Further, Volvo continued to support the development work of the various E4 Mistra system project components such as LNC catalysts, reformer catalysts, sintered metal particulate filter and thermo electric generator. To support the work with the reformer catalysts, Volvo together with KTH performed a reactor study at VTEC to evaluate the performance of Manganese (Mn) containing reformer catalysts with reduced amounts of precious metals. The purpose of performing the tests at Volvo is to evaluate these catalysts in another reactor set-up and with other gas analysis instrument in order to capture phenomenon only related to catalytic processes and not to reactor system components and design. The study showed that Mn-promoted catalysts with reduced precious metal loading (compared to standard reference) had a good diesel reforming capacity although less than the reference catalyst, but still high enough to be considered as an interesting candidate which is worth a further investigation and preparation optimization.

To support the development of LNC catalysts, Volvo together with KCK evaluated the $NO_x$ conversion performance of a series of $Ag/Al_2O_3$ catalysts with different Ag loadings. The catalysts are prepared using the sol-gel method, but are further optimized to improve low temperature activity. Both low sulphur diesel and biodiesel (NExBTL) were used as reducing agents in this study. The effect of hydrogen traces on the performance of the LNC catalysts was also included in this study.

To support the development work of sintered metal particulate filter, Volvo has built a system to investigate soot and ash loading behaviour of this filter. During 2011, Volvo has purchased a diesel fueled generator system (gen-set) with a power capacity of 5 kW. The gen-set is used as exhaust gas generator. In addition to the diesel gen-set, the soot and ash loading set-up consists of an electric heater which is used to heat the exhaust from the gen-set when needed, a diesel oxidation catalyst to increase the exhaust gas temperature

for DPF regeneration, the Höganäs DPF with the filter holder and a heat exchange to cool the exhaust gas in the DPF outlet before sending the gas to ventilation. To shorten the testing of the DPF capacity for ash loading, accelerated ash loading tests are performed by oil doping in the diesel used in the combustion process.

To support the work with thermo electric materials and thermo electric generators, Volvo is leading team discussion meetings which gather all involved project participants from TYK, KRT, Alfa Laval and Termo-Gen. During the meetings technical issues and challenges are discussed and actions are taken for forward movement in the development process. Volvo is also providing technical support whenever engine system data are required.




5 kW gen-set system used for evaluation of component projects.

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This component is performed by Jazaer Dawody, Lennart Andersson, Miroslawa Milh, Timothy Benham, Mikael Ohlsson and Jan Koegler at Volvo Technology.

# Communication of results

The results of the programme are summarized in internal reports. Results have also been presented at conferences, scientific journals and theses.

## Conference contributions and presentation

1. X. Karatzas, K. Jansson, A. González, J. Dawody, and L.J. Pettersson Autothermal reforming of low sulphur diesel over bimetallic RhPt supported on $Al_2O_3$, $CeO_2$-$ZrO_2$, $SiO_2$ and $TiO_2$. Proceedings of the 22nd North American Catalysis Society Meeting, Detroit, MI, June 5-10, 2011.
2. D. Creaser, X. Karatzas, B. Lundberg, L.J. Pettersson, and J. Dawody. Modeling Study of 5 kWe-Scale Autothermal Diesel Fuel Reformer. Proceedings of the 22nd North American Catalysis Society Meeting, Detroit, MI, June 5-10, 2011.
3. M. Z. Granlund and L.J. Pettersson. Assessing the influence on activity by adding Mn to diesel autothermal reforming catalysts. Proceedings of the Ninth European Congress on Catalysis EUROPACAT X, Glasgow, United Kingdom, 28 August – 2 September, 2011.
4. F. Gunnarsson, H. Kannisto and H. H. Ingelsten. The influence of trace-amount PM-doping on lean $NO^x$ reduction by HC-SCR over $Ag/Al_2O_3$. 22st North American Catalysis Society Meeting (22th NAM), Detroit, USA, June 5-10, 2011.
5. H. Kannisto, X. Karatzas, J. Edvardsson, L. J. Pettersson and H. H. Ingelsten. Lean NOx reduction over $Ag/Al^2O^3$ – an on-board system approach. 22st North American Catalysis Society Meeting (22th NAM), Detroit, USA, June 5-10, 2011.
6. H. H. Ingelsten, A. Hellman, H. Kannisto and H. Grönbeck. Combining DRIFT and DFT to characterize $NO_x$ species on $Ag/\alpha$-$Al_2O_3$. 22st North American Catalysis Society Meeting (22th NAM), Detroit, USA, June 5-10, 2011.
7. M. M. Azis, H. H. Ingelsten and D. Creaser. Promotional effect of $H_2$ on NO oxidation over Ag-$Al_2O_3$. 22st North American Catalysis Society Meeting (22th NAM), Detroit, USA, June 5-10, 2011.
8. K. Arve, H. Kannisto, H. H. Ingelsten, K. Eränen, M. Skoglundh and D. Y. Murzin. $O_2$ chemisorption and TEM imaging for determination of silver mean particle size, distribution and oxidation state of $Al_2O$. EuropaCat X, Glasgow, Scotland, August 28-September 2, 2011.
9. M. Männikkö, M. Skoglundh and H. H. Ingelsten. Effect of $H_2$ and C/N on methanol-SCR over supported Ag catalyst. EuropaCat X, Glasgow, Scotland, August 28-September 2, 2011.
10. A.E.C. Palmqvist. Improvement of thermoelectric materials by nanoinclus- ions, UCSB-Chalmers Workshop on Materials for Energy Applications, Santa Barbara, USA, April 4-5, 2011.
11. Y. Ma, E. Ahlberg, Y. Sun, B. Brummerstedt Iversen and A.E.C. Palmqvist. Characterization of the thermoelectric properties of electrodeposited thin films of telluride compounds. European Workshop on Electrochemical Deposition of Thermoelectric Materials, Kaub, Germany, April 11-12, 2011.
12. Y. Ma, W. Wijesekara, E. Ahlberg, Y. Sun, B. Brummerstedt Iversen and A.E.C. Palmqvist. Characterization of the thermoelectric properties of electrodeposited thin films of telluride compounds. 30th International Conference on Thermoelectrics (ICT 2011), Traverse City, Michigan, USA, July 17-21, 2011.
13. R. Heijl, D. Cederkrantz, M. Nygren, and A.E.C. Palmqvist. Thermoelectric properties of $Ba_8Ga_{16}Ge_{30}$ clathrate with $TiO_2$ nanoinclusions. 30th International Conference on Thermoelectrics (ICT 2011), Traverse City, Michigan, USA, July 17-21, 2011.
14. D. Cederkrantz, M. Søndergaard, M. Christensen, B.B. Iversen, and A.E.C. Palmqvist A comparison between the laser flash method and the transient plane source technique for thermal conductivity measurements. 30th International Conference on Thermoelectrics (ICT 2011), Traverse City, Michigan, USA, July 17-21, 2011.
15. A.E.C. Palmqvist. Bringing nanostructured thermoelectrics to use in waste heat recovery for vehicles. Seminar on Thermoelectrics for future energy management, IVA, Stockholm, Sweden, September 15, 2011.
16. A.E.C. Palmqvist. Improved thermoelectric performance by introduction of nanoinclusions. at Nanomax Workshop, Stockholm, Sweden, October 18, 2011.

17. A.E.C. Palmqvist. Bringing nanostructured thermoelectrics to use in waste heat recovery for vehicles. Nanothermoelectrics Workshop and Networking Meeting, Lund, Sweden, October 26, 2011.
18. O. Högblom and R. Andersson, CFD Modeling of Thermoelectric Generators in Automotive EGR-coolers. 9th European Conference on Thermoelectrics, Thessaloniki, Greece, September 28-30, 2011
19. J. Edvardsson. E4 Mistra, fas 2 -Energieffektiv rening av avgasemissioner från fordon. Energirelaterad fordonsforskning, Örebro, Sweden, November 2-3, 2011.
20. L.J. Pettersson. Putting chemical engineering in the driver´s seat: Catalytic solutions for solving emission and efficiency problems in the automotive sector for 2020 and beyond. Anders Holmen seminar, Trondheim, Norway, 2 December, 2011.

## Peer-reviewed papers

1. X. Karatzas, J. Dawody, A. Grant, E. E. Svensson and L. J. Pettersson. Zone-coated Rh-based monolithic catalyst for autothermal reforming of diesel. Appl. Catal. B. 101 (2011) 226-238.
2. X. Karatzas, D. Creaser, A. Grant, J. Dawody and L. J. Pettersson. Hydrogen generation from n-tetradecane, low-sulphur and Fischer-Tropsch diesel over Rh supported on alumina doped with ceria/lanthana. Catal. Today 164 (2011) 190-197.
3. H. Kannisto, X. Karatzas, J. Edvardsson, L.J. Pettersson and H.H. Ingelsten. Efficient low temperature lean NOx reduction over Ag/Al2O3 – Optimization of a possible on-board system. Appl. Catal. B 104 (2011) 74-83.
4. X. Karatzas, J. Dawody, A. González and L.J. Pettersson. Autothermal reforming of low-sulphur diesel over bimetallic RhPt supported on $Al_2O_3$, $CeO_2$-$ZrO_2$, $SiO_2$ and $TiO_2$. Appl. Catal. B 106 (2011) 476-487.
5. D. Creaser, X. Karatzas, B. Lundberg, L.J. Pettersson, and J. Dawody. Modeling Study of 5 kW -Scale Autothermal Diesel Fuel Reformer. Appl. Catal. A 404 (2011) 129-140.
6. X. Karatzas, K. Jansson, J. Dawody, R. Lanza and L.J. Pettersson. Microemulsion and incipient wetness prepared Rh-based catalyst for diesel reforming. Catal. Today 175 (2011) 515-523.
7. K. Arve, H. Kannisto, H. H. Ingelsten, K. Eränen, M. Skoglundh and D. Y. Murzin. Did chemisorptions become an obsolete method with advent of TEM? Comparison of mean particle size and distribution of silver on alumina. Catal. Lett. 141(5) (2011) 665.
8. Y. Ma, E. Ahlberg, Y. Sun, B. B. Iversen and A. E. C. Palmqvist. Thermoelectric properties of thin films of bismuth telluride electrochemically deposited on stainless steel substrates. Electrochimica Acta, 56 (11), (2011), 4216-4223.
9. Y. Ma, E. Ahlberg, Y. Sun, B. B. Iversen and A. E. C. Palmqvist,Thermoelectric Characteristics of Electrochemically Deposited $Bi_2Te_3$ and $Sb_2Te_3$ Thin Films of Relevance to Multilayer Preparation. J. Electrochem. Soc. 159 (2), (2012), D50-D58.
10. D. Cederkrantz, N. Farahi, K. A. Borup, B. B. Iversen, M. Nygren and A.E.C. Palmqvist Enhanced thermoelectric properties of $Mg_2Si$ by addition of $TiO_2$ nanoparticles. J. Appl. Phys. 111, (2012) 023701.
11. Y. Ma, W. Wijesekara and A.E.C. Palmqvist. Electrochemical Deposition and Characterization of Thermoelectric Ternary $(Bi_xSb_{1-x})_2Te_3$ and $Bi_2(Te_{1-y}Sey)_3$ Thin Films. J. Electronic Mater, (2012) DOI: 10.1007/s11664-011-1790-y.

## Master theses

1. Jenny-Yue Zheng. Silver-alumina catalysts for lean $NO_x$ reduction: Influence of hydrothermal ageing. Chalmers University of Technology, Gothenburg, 2011.
2. Nader Farahi. Thermoelectric nanocomposites. Chalmers University of Technology, Gothenburg, 2011
3. Waruna Dissanayaka Wijesooriyage. Electrochemical deposition and characterization of thermoelectric thin films of $(Bi_xSb_{1-x})_2Te_3$. Chalmers University of Technology, Gothenburg, 2011
4. Pham Hoang Ngan. Gold nanoinclusions in thermoelectric germanium clathrates. Chalmers University of Technology, Gothenburg, 2011

## Theses

1. Yi Ma. Electrochemical deposition and characterization of thermoelectric thin films of bismuth telluride and its derivatives. Chalmers University of Technology, Gothenburg, 2011.
2. Xanthias Karatzas. Rhodium diesel-reforming catalysts for fuel cell applications. Royal Institute of Technology, Stockholm, 2011

# Management and organization of E4-Mistra

The programme is a joint research initiative between four academic partners and four industrial partners:

Chemical Engineering and Technology, Royal Institute of Technology (KTH)
Competence Centre for Catalysis, Chalmers University of Technology (Chalmers)
Applied Surface Chemistry, Chalmers University of Technology (Chalmers)
Chemical Reaction Engineering, Chalmers University of Technology
Volvo Technology AB
Termo-Gen AB
Höganäs AB
Alfa Laval AB
Volvo Technology AB hosts the programme. The board has overall responsibility for the programme. The board members during 2011 were:

Thomas Johannesson (Chairman), former Dean of LTH, Lund University
Ove Backlund, former head of Advanced Engineering Engine section at Volvo Car Corporation, Sweden.
Gunilla Jönsson, Senior Professor in Packaging Logistics, Lund University;
Kersti Hermansson, Professor at Uppsala University
Bo Leckner, Professor emeritus in Energy Conversion at Chalmers University of Technology.
Owe Mårs, Manager Alloy Development Surface Coating, Höganäs AB.
John Korsgren, Advanced engineering coordinator for Exhaust Aftertreatment, Volvo Powertrain AB
Mats Nilsson, R & D Manager, Alfa Laval AB
Christopher Folkeson Welch (co-opted member), Programmes Director at Mistra

# Management team

Jonas Edvardsson has during 2011 replaced Heije Westberg as the programme director. Heije Westberg remains in the programme as deputy programme director. The programme director together with the respective project leaders constitute the management team.

The project leaders are:
Hanna Härelind Ingelsten, Assoc. Prof., Competence Centre for Catalysis, Chalmers.
Lars J. Pettersson, Prof., Department of Chemical Engineering and Technology, KTH
Anders Palmqvist, Prof., Applied Surface Chemistry, Chalmers.
Ronnie Andersson, Assist. Prof., Chemical Reaction Engineering, Chalmers
Jazaer Dawody, Ph.D., Exhaust Aftertreatment and Fuel Reforming, Volvo Technology AB
Per-Olof Larsson, Ph.D., Manager, Global development/filters, Höganäs AB
Lennart Holmgren, Mr., Managing director of Termo-Gen AB.
Fredrik Andreasson, Mr., Concept development, Alfa Laval AB

One programme meetings for all programme participants including the programme board was held near Skövde in September 2011, and a system integration workshop was held in Göteborg in March 2011.

Jonas Edvardsson

Heije Westberg

## Budget

| | 2011 | Total |
|---|---|---|
| Mistra funding | 5.84 | 24.00 |
| Catalytic $NO_X$ reduction | 1.14 | 4.75 |
| Reformers for $H_2$ production | 1.16 | 4.75 |
| CFD for heat exchangers | 0.81 | 2.35 |
| Thermoelectric materials | 1.19 | 4.75 |
| Reserve | 0.75 | 3.0 |
| Management | 1.06 | 4.4 |
| FFI funding | 2.7 | 10.0 |
| In-kind contribution | 3.8 | 14.0 |
| Höganäs AB | 1.60 (0.56)* | 4.5 (1.57) |
| Termo-Gen AB | 1.49 (0.75) | 6 (3.0) |
| Alfa Laval AB | 1.11 (0.56) | 4 (2.0) |
| +Volvo Technology AB | 2.30 (0.83) | 9.5 (3.42) |

*) The amount in parenthesis is funding from FFI

Participants at the program meeting in Gotland, August 2010

From left to right: Olle Högblom, Ronnie Andersson, Lars Pettersson, Lennart Holmgren, Thomas Johannesson, Moa Zithén Granlund, Hanna Härelind Ingelsten, Bengt Andersson, Ove Backlund, Anders Palmqvist, Per-Olof Larsson, Richard Heijl, Britt Marie Bertilsson, Heije Westberg, Lennart Andersson, Fredrik Gunnarsson, Jonas Edvardsson, Ma Yi, Owe Mårs, Mats Nilsson

MISTRA in brief

## Research with practical benefits

The Swedish Foundation for Strategic Environmental Research – Mistra - supports research of strategic importance for a good living environment and sustainable development.

It invests in research groups who, working alongside users, are able to contribute to solving major environmental problems.

Mistra's programmes cut across disciplinary boundaries, and the results are intended to find practical applications in companies, public agencies and non-governmental organizations.

Mistra provides funding for some twenty major programmes, each extending over six to eight years. All of them have the aim of building bridges, both between disciplines and between researchers and users.

The Foundation's strategy is to seek to ensure that its funds produce a threefold return: strong research environments that create value for users, asset management in support of sustainable development, and active communication to make the results known.

Further information can be found on our web site:

**www.mistra.org**