



Working Paper

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Publication Date:

2002

Permanent Link:

<https://doi.org/10.3929/ethz-a-004261270> →

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PSI Bericht Nr. 02-02

Januar 2002

ISSN 1019-0643

General Energy Department (ENE)

The Role of Chemical Processes in the Transition to Sustainable Energy Systems

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Chemical science and engineering play a central role in improving the eco-efficiency of energy services, be it by optimizing fossil fuel utilization from the source to the sinks, be it by exploring new ways of replacing fossil fuels with renewable ones. Catalytic fuel processing is required for providing clean and easy to convert inputs from contaminated and/or high molecular weight primary resources into efficient energy conversion systems such as advanced combustion engines and fuel cells. The switch from conventional fossil fuel resources to renewables such as solar or biomass requires new approaches in chemical engineering. Efficiency vs. emissions trade-offs for improving the eco-performance of combustion engines need to be optimized with improved understanding of the complex chemistry taking place in flames. New materials for fuel cells and batteries provide a means of making these devices applicable, thereby drastically cutting down on emissions from energy systems. Chemistry is not only involved in fuel processing and conversion, but it is also important at the end of the pipe, i.e. in catalytic emission control devices, in the treatment of hazardous residues from the incineration of waste materials, and in the complex interactions of air pollutants with the biosphere.

1. Introduction

The availability of energy in sufficient quantity and quality has been a prerequisite for a thriving economy. Energy consumption in developing economies correlates directly with the standard of living of its inhabitants, as indicated by a country's GNP or other equivalent indicators [1]. On the other hand, our use of energy stresses the environment through local pollution, emission of greenhouse gases (e.g. CO₂, methane and N₂O) and global warming. While developing countries experience the positive impact of increased energy availability on their standard of living, we clearly have reached the point in industrialized societies of diminished benefits from increased energy consumption. Energy as a motor for development and at the same time as a global threat to the environment has become a source of conflict and it has proved difficult to define and adhere to common goals. The vision of sustainable development may require dramatic re-partitioning of energy

resources.

An ambitious goal formulated [2] with a view to sustainability is that global energy consumption should not increase at a higher rate than the world population, in spite of substantial economic development taking place in several world regions. To achieve this aim, the global average of primary energy consumed per person and year, equivalent to an energy flux per person of 2000 W, must not be exceeded. This is a factor of ≈ 3 above what an average inhabitant of Africa is consuming today, and it is a factor of 5 below what an average North American is consuming. Whether we will be able to reduce primary energy input by the factors required in industrialized countries by improving efficiency of production and use of energy, or whether we will have to cut back in our end-use, is a controversial question.

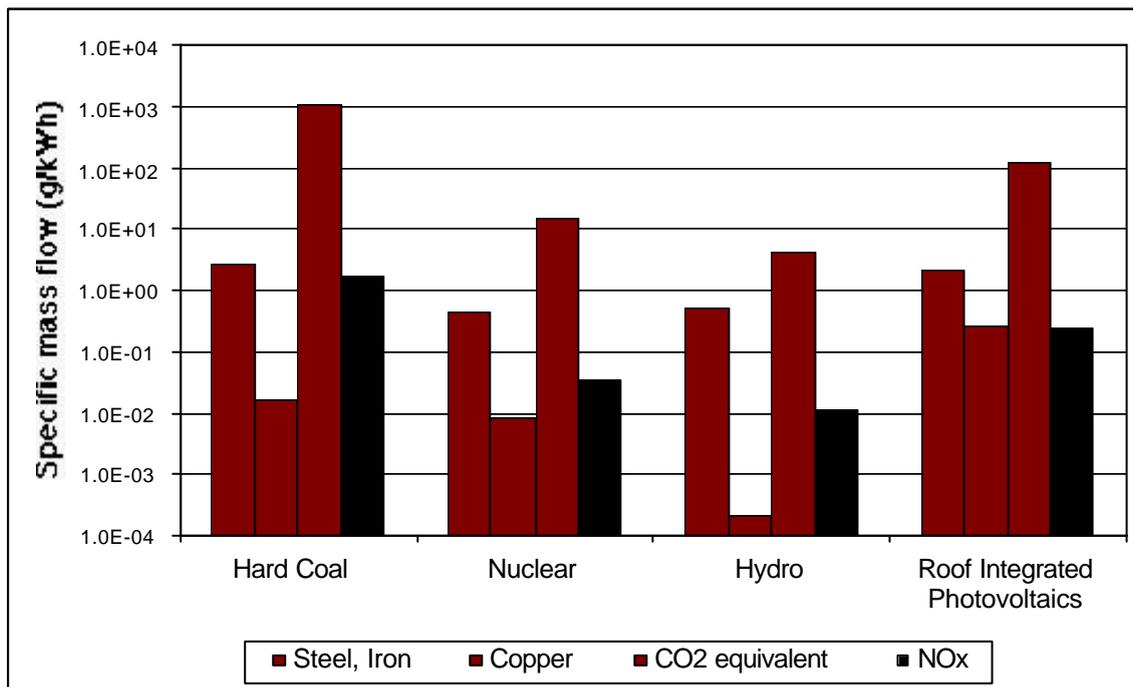


Figure.1: Total life cycle mass flows of selected materials and emissions involved in providing 1 kWh of electric power from the full energy chains of hard coal, nuclear, hydro, and photovoltaics (integrated on roofs in central European location) using present average power plant technology in Europe (UCPTE countries). Graph based on data from Frischknecht et al. [3].

It is important, however, to recognize that, on a global average, energy fluxes from human activities are three to four orders of magnitude lower than the energy flux of the sun to the

earth. Therefore, by themselves, they are not relevant for the energy balance of the globe. Energy use is, however, an environmental problem because of the *material flows*

(resource use, transport, waste, pollutants, greenhouse gases) associated with the way energy is collected, converted, and consumed today. To illustrate this, figure 1 shows a selection of material flows which are induced to provide 1 kWh of electric power for four different power-generating technologies. It takes into consideration the full energy chains, i.e. from mine to waste disposal, over the entire lifetime of all the facilities involved. All technologies involve substantial flows of materials and emissions, depending on the fuel base of the technology (e.g. coal vs. nuclear) or the power densities and the resulting material intensities involved in the energy conversion plants (low power density of sun light creates high material intensity for photovoltaic power generation). It is important to note that all the power-generating technologies cited in figure 1 lead to emissions of greenhouse gases, even if they operate on non-fossil resources. This is due to the fact that, to be consistent, energy inputs into the erection of plants, equipment, transport, as well as the resulting emissions are calculated on the basis of today's energy mix.

Figure 1 illustrates clearly that, although the tapping of any primary energy involves material flows for setting up the necessary infrastructure, it is mainly our predominant carbon based fossil fuel economy which involves huge material flows into the environment. Globally, the combustion of oil, gas, and coal emits 22 Gt of CO₂ to the atmosphere annually. With the Gigatons of CO₂ emissions globally, energy conversion can be viewed as the industry with the largest volume of chemical output. (e.g.: Switzerland which produces its electric power from hydro and nuclear plants, still "produces" 44 Mt/y of CO₂ from burning fossil fuels compared to 3.5 Mt/y of cement, and 2.6 Mt/y of municipal solid waste). Given this situation, it is clear that chemistry and chemical engineering have to play a central role in solving the problems associated with energy use. The development of the oil industry over the past 50 years to its leading position in the present energy market has been strongly linked with advances in chemical engineering science. With the huge

capacities of its refineries and petro-chemical plants, the oil industry has become the pace-maker in chemical engineering research. The transition away from the predominant dependence on oil will need a dramatic breakthrough in the field of chemical engineering for energy conversion, eventually leading to a better chemistry for energy conversion, involving less material flows and less pollution.

Chemical fuels are the form of energy which has been dominating the market ever since the Industrial Revolution took off: Worldwide, about 80% of commercial and non-commercial energy today is based on chemical fuels (coal, petroleum, natural gas and fuel-wood). The conversion of these fuels in combustion processes provides mechanical work, lighting or heat, i.e. the classical energy services. Fuels can be stored and, thanks to this fact, make energy use temporally and spatially independent of the abundant but uncontrollable natural energy fluxes from the sun and its secondary forms, i.e. wind- or water-power. This is why fossil fuels and the development of thermal engines have been so successful in fuelling the Industrial Revolution: With fossil fuels providing the energy for producing electric or mechanical power the grain can be milled when there is demand for flour and not only when there is wind or water...

The transformation of fossil resources into fuels or chemical feedstocks, as well as their combustion for delivering energy services, are chemical processes which run with more or less efficiency, product yield and selectivity. Good practice in the conversion of primary energy to ready-to-use fuels and of fuels to heat and/or electric power requires mastery of the chemistry involved in a way which minimizes the losses via side products as unwanted emissions or as lost energy.

The dramatically increased use of fossil resources has led to the well-known pollution problems which endanger environmental and human health on a local and on a global level. Furthermore, they have become one of the central problems to be solved in the context of sustainable development.

The global problem of fossil fuels: CO₂

On the global level the environmental impact of fossil fuels burning is connected with feeding excess carbon at an unprecedented rate into the natural carbon cycle. As a result we find an accumulation of carbon dioxide in the atmosphere leading to 1) global warming

effects (greenhouse effect) and 2) prospective direct impacts on the biosphere, like changes in the water management of plants leading to local secondary climatic impacts. The emission of CO₂ with its global effects on climate and its impact on vegetation is intrinsically connected with the material basis

of today's fuels: CO₂ is the waste product of the fossil fuel chain and can not be avoided unless the fuel chain is changed dramatically. Strategies for reducing the emissions of CO₂ for a given energy service include:

- **Sufficiency:** Reducing the amount of energy services by basically adopting a different life-style. This strategy requires fundamental changes in cultural values and social attitudes. This very important strategy is acknowledged to be central for reaching sustainability in the long term. It is, however, beyond the scope of the present article.
- **Efficiency:** Increasing the efficiency of the fuel conversion chain, from the source to the end-use. This strategy is expected to have potential of reducing substantially the input of primary energy for equal energy services. A recent study carried out for Switzerland identified reduction potentials for fossil fuels by improved efficiency between 20% (for the household sector)

The local problem of fossil fuels: air pollutants

On a local level, most combustion processes lead to side products, other than the main products CO₂ and water. The side products include molecular species such as nitrogen oxides, CO, unconverted hydrocarbons (VOC) or aerosol particles of soot and/or ash. Some of the side products are very reactive and lead to complex secondary reactions in the environment, some are very persistent and can have detrimental effects by their accumulation in the atmosphere, or in the food chain.

Local pollutants arise if fuels are being burnt which contain elements other than C and H. Sulfur and nitrogen in fuels can lead to acidic emissions. Furthermore minerals and heavy metals in the fuels can lead to toxic particulate emissions.

These emissions have to be avoided by either processing the fuels prior to combustion, or by scrubbing the combustion gases prior to releasing them to the environment. Both operations lead to the accumulation of solid residues which need further treatment for safe disposal.

Local pollutants can also arise from incomplete or uncontrolled reaction of the fuel with combustion air. These side products of the combustion process, such as aerosol particles (also particulate matter, PM), thermal NO_x, CO, and VOC, can be reduced by

and 50% (in transportation) by the year 2020 [4] relative to the 1990 values.

- **Decarbonised fuels:** Switching to low carbon fuels, by e.g. substituting coal by natural gas for power generation, or to zero carbon fuels like solar hydrogen;
- **Carbon recycling:** Strategies to make use of the advantages of carbonaceous fuels (easy handling and storage) in a sustainable way by tapping renewable sources of carbon, like biomass;
- **Carbon sequestration:** Finding ways of processing fossil fuels such that concentrated CO₂ can be recovered and disposed of safely, "out of the reach of the atmosphere", e.g. in the deep ocean.

All but the first of these strategies involve chemical know-how and can be aided by research into the underlying chemical processes.

improved energy conversion techniques (staged combustion, catalytic combustion, cold combustion in fuel cells), or by appropriate gas clean-up technologies in the exhaust stream, including catalytic converters for NO_x and CO, and particulate filters. However, the available reduction technology is often not implemented due to cost considerations.

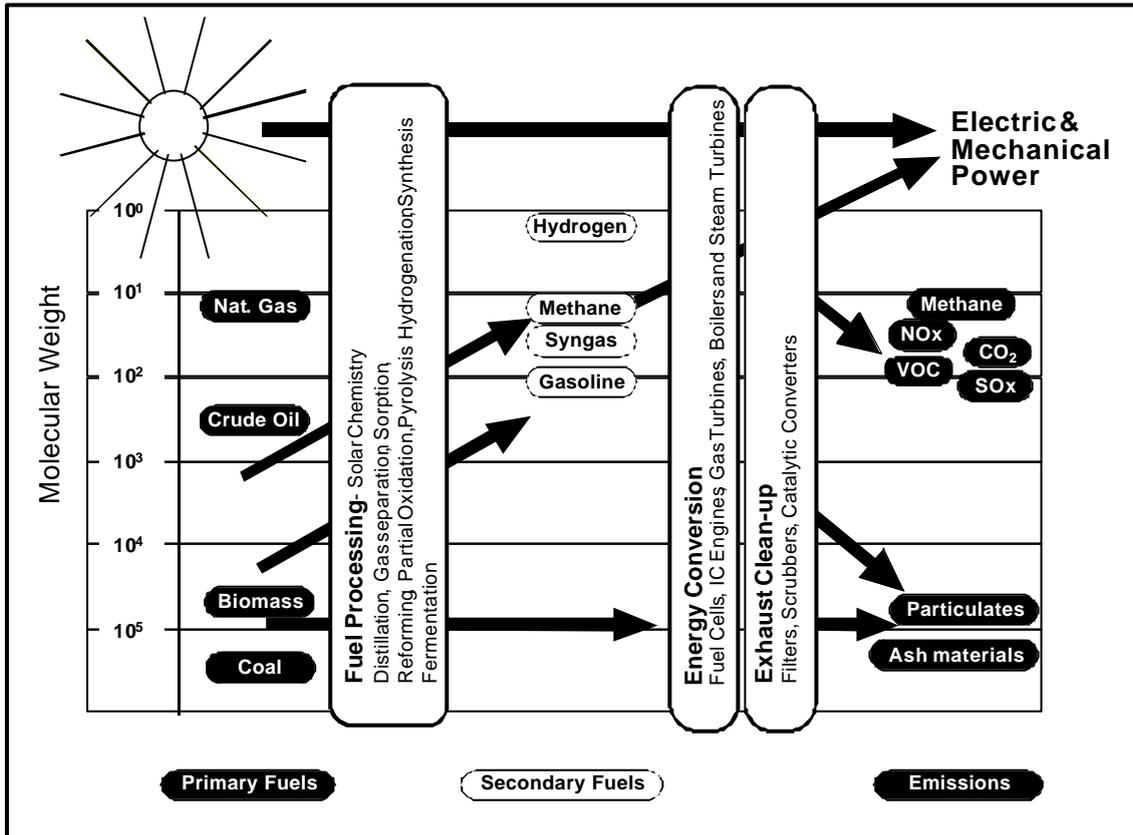
Once in the atmosphere, the pollutants can directly have adverse health effects. Especially small particles are important because they penetrate into the lungs of humans. Epidemiological studies have clearly shown a relationship between increased aerosol mass concentrations, respiratory health problems and enhanced mortality. Benzene and other compounds are known to be carcinogenic. By photochemical reactions in the air, secondary pollutants like ozone may be formed that are known to affect both humans and the biosphere to a considerable extent.

Furthermore, aerosol particles are exerting a cooling effect on climate, both by scattering light back to space and by changing the albedo of clouds. This effect, which is still very poorly quantified, may result in a considerable masking of the effect of the greenhouse gases. Better data are therefore needed in order to provide a comprehensive modeling of the integrated effects of fuel combustion on our climate.

Similar to elevated CO₂, air pollutants directly affect the vegetation cover too. Like ozone, which causes a considerable crop loss, nitrogen compounds (NO_x, NH₃ etc.) induce changes in plant growth and in the efficiency of water use, resulting in a lowered stress resistance and ecosystem stability.

For these reasons, sustainable development strategies have to include environmental impact considerations (see

below).



2. From primary fuels to energy services: chemical processes along the fuel chain

Figure. 2: From fuels to energy services. Gaseous fuels give best conversion efficiencies and lowest emissions. Fuel processing: Conversion of high molecular weight fuels such as biomass or coal to low molecular weight fuels. Energy conversion: fuel properties decide on appropriate technology. Exhaust clean-up is more demanding for the combustion of dirty fuels.

Society relies on a multitude of fuels for providing the energy services required: Fuel qualities differ with respect to state of aggregation (liquid, gaseous, solid), purity, chemical and physical homogeneity, pollution potential upon conversion, handling and transportation (spilling), conversion value (ease of achieving high conversion efficiency), and logistic manageability. In order to reduce the environmental impact of fuel burning, most

available fuels need to be processed prior to the energy conversion, or else the combustion products require downstream processing, i.e. exhaust treatment, or both.

Figure 2 gives an overview of the process steps along the fuel chain. Primary energy resources need, in most cases, to be processed prior to use in energy conversion processes. Fuel processing means in most cases reducing the molecular weight of the fuel

compounds for optimizing the subsequent energy conversion processes and for removal of pollutants. Highly efficient and clean energy conversion devices, such as advanced gas turbines or fuel cells, require low molecular fuels for best performance. In this sense, hydrogen, directly derived from solar energy and water is the ultimate fuel with respect to optimized efficiency and cleanliness, if economically acceptable ways of producing it will be made available. In order to minimize the environmental impact of energy conversion processes, air pollution control technology is either integrated into the combustion process, or added as an after-treatment. All these processes for providing fuels from depletable or renewable resources and their conversion to useful energy involve chemistry and chemical engineering. Finally there is a host of chemical processes taking place in the environment due to the substances emitted by the fuel chain. An overall optimization of these processes is crucial for improving the ecological and economic performance (eco-efficiency) of

energy services. The concept of eco-efficiency has been defined by the World Business Council for Sustainable Development as follows: "Eco-efficiency is reached by the delivery of competitively priced goods and services that satisfy human needs and bring quality of life while progressively reducing ecological impacts and resource intensity through the life cycle, to a level at least in line with the earth's estimated carrying capacity"[5]. In the context of chemistry of the fuel chain, eco-efficiency means optimizing the chemical processes in the fuel processing, fuel conversion and post treatment steps and choosing the best chains for a given application, taking into account the environmental impact as well as the economic constraints. There are trade-offs to be made between investing into high performance fuel processing, energy conversion, or post-treatment. The decision can only be supported by an environmental and economic analysis covering the whole life cycle of all the process steps involved (LCA).

2.1. Fuel production and processing

Fuel processing involves chemical transformations and physical separations of primary fuels (fossil or biomass) to secondary fuels for energy conversion:

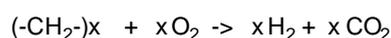
- pyrolysis or thermal cracking is applied for converting heavy liquid and solid fuels (coal, heavy distillation residues, biomass) into mixtures of liquids, gases and residual carbon ("char");
- catalytic or non-catalytic partial oxidation for breaking down complex carbonaceous fuels to low molecular weight combustible gases (typically H₂, CO₂): gasification of solid fuels (coal, biomass), partial oxidation of distillation residues in refining, partial oxidation of liquid transportation fuels for on-site production of hydrogen;
- reforming, i.e. endothermic reaction of carbonaceous fuels with steam or CO₂, producing mixtures of combustible gases;
- enzymatic conversion of biomass to methane or alcohol in bio-reactors (fermentation);
- separation technologies, such as distillation, desulfurization, removal of alkali or heavy metals, removal of inert components such as CO₂, etc., by solvent absorption (scrubbing) or by adsorption (e.g.: pressure swing adsorption, PSA).

The most important chemical reactions in fuel processing are partial oxidation and reforming, processes which run at high temperatures in order to overcome kinetic restrictions. There is incentive to run such processes at the lowest possible temperatures in order to minimize heat losses, i.e. in order to improve the efficiency of the process. Temperatures can be significantly lowered and selectivities of reactions improved by running these processes over heterogeneous catalysts [6].

The distributed production of hydrogen for providing the fuel for fuel cell power generators is likely to be of central importance for the introduction of fuel cells for stationary and mobile applications before pure hydrogen will be available as the standard gaseous fuel in the far future. Endothermic steam reforming of liquid fuels produces hydrogen, both from the liquid hydrocarbon or alcohol, and from the added steam:



This reaction involves water splitting and is highly endothermic. The reaction enthalpy can be provided by the exothermic partial combustion of additional fuel:



In a suitable catalytic reactor, partial oxidation and reforming of the fuel can be combined such that the overall reaction is thermally neutral. The chemical engineering challenge is to manage the endothermic and exothermic parts of the overall reaction such that local temperature deviations (hot and cold spots) are minimum. Selectivity of the reaction to CO_2 and H_2 as products is the central problem in devising a fuel processor for the PEM fuel cell. Low levels of CO (above 50 ppm) are very detrimental to the efficiency of the fuel cell and must be avoided. Practical reformers and partial oxidation catalysts produce CO levels which need further processing of the gas (membrane separation of hydrogen, or preferential specific oxidation of the remaining CO in a second catalytic stage).

Partial oxidation and reforming can be applied to any kind of carbonaceous fuel, including solids such as coal, lignite or wood. The proven reserves of coal are far more abundant than those of petrol which means that, in the mid term, technologies for converting solid fuels to liquids will become increasingly important. Enhanced mining and use of coal will, however, not be in line with a policy aiming at stabilized or reduced CO_2 emissions. Biomass is, in contrast, a renewable source of carbonaceous fuel, as long as it is managed in a sustainable way (i.e. not more is harvested from a given area than can be regrown in an annual vegetation cycle).

For the conversion of solid biomass, partial oxidation is commonly referred to as auto-thermal gasification, reforming as steam gasification. In autothermal gasification, a solid fuel is reacted in a suitable solid-gas reactor with air or oxygen as the gasification agent at temperatures above 800°C . The challenge in biomass gasification is the production of synthesis gas (a mixture of CO , H_2 , CO_2) with no or little other components. The spectrum of side products again depends on the gasification technology chosen. The side products include methane, tars and particles. Tars are condensable hydrocarbons which result from the breakdown of the solid fuel in pyrolysis ("primary tars") and reaction products of these primary products to more stable secondary products ("secondary tars"). The range of tar components which form in a gasification process depend critically on the composition of the primary biomass fuel [7]. Tars can be eliminated by down-stream processes such as catalytic or thermal cracking of the raw gas. In large facilities for converting biomass to syngas this can be done using more or less standard technology. An assessment of the technological and economic implications of the gas processing

steps required for the conversion of woody biomass to methanol has been made in a feasibility study [8].

The feasibility of thermal conversion of biomass to pure and high value chemical fuels such as methanol has so far been limited to studies for large scale conversion plants. Large scale in the field of biomass conversion is typically in the range of 20 MW up to a maximum of 100 MW which is small if compared with typical petrochemical plants which are in the order of 1000 MW. The distributed nature of biomass (yields ranging from 50 GJ per hectare and year for forestry to 1000 GJ/ha and year for intensive sugar cane plantations) and the resulting transportation distances (up to 100 km radius) are limiting the plant size. Conventional conversion technologies have been borrowed from coal and petroleum technologies, but the substantial economy of scale for such plants cannot be exploited for the reasons given above. The processing of wood to high quality fuels with good conversion efficiency and at competitive costs in relatively decentralized plants is therefore still an unsolved problem. New ideas are required to handle the difficult chemistry of pyrolysis and gasification and subsequent product upgrading on small, distributed scale.

Separation technologies are necessary to remove species which later in the fuel chain might lead to emissions or which might interfere with the energy conversion step or cause more cost in the final exhaust clean-up steps. Separating hetero-elements from a simple fuel such as natural gas or liquid hydrocarbons can be made cost-effectively (desulfurization processes in refinery processes) in the fuel processing stage, whereas with complex solid fuels (biomass, coal, waste) the separation process is better performed after gasification or after the combustion step (see below).

Separation at high temperature is a central issue in high temperature solar chemistry for producing hydrogen from water and concentrated solar radiation via metal oxide cycles. This emerging technology - the ultimate fuel processing technology - will succeed if the products from thermal dissociation reactions at very high temperatures can be separated efficiently and prevented from back reaction.

The emerging field of high temperature solar chemistry research is exploring the potential of producing fuels with sunlight, and of substituting high temperature process heat for fossil fuels in industrial processes leading to material commodities like Zn, Al, syngas,

cement, etc.[9-12] The goal from both activities is to develop science and technology for reducing society's demand for fossil. The work is focused on the development of solar chemical reactors that operate at temperatures from 1200 - 2200 K. Physical chemistry questions with regard to the mechanisms and rates of decomposition and re-oxidation reactions are being investigated [13,14]. Techniques are being developed that enable one to ascertain material properties and temperatures under intense solar radiation. [15] Models are emerging that combine radiation heat transfer, chemical kinetics, as well as mass and energy conservation principles so that one can predict a solar chemical reactor's output as a function of its solar input. Reactors from 5 kW up to near 0.5 MW are being designed and tested. [10-12]

An example of a sunlight to fuels process under investigation is the development of a process for the direct thermal decomposition of ZnO to its elements.[9] In this process, concentrated sunlight provides high-temperature process heat for the endothermic reaction



2.2. Energy conversion processes:

2.2.1. Combustion technology

Combustion engines are the dominant conversion devices to transform chemical fuels into useful mechanical energy. With the exception of electric trains, virtually 100% of land, sea and air transportation relies nowadays on combustion engines. A major portion of electricity worldwide is produced by thermal processes based on combustion technology as well.

The main challenge in combustion science is the simultaneous optimization of the parameters affecting the thermodynamic process efficiency and minimization of polluting components in the exhaust gas (mainly nitrogen oxides, soot particles and unburned hydrocarbons). As an important step in this direction, we have recently realized [17] a natural gas engine for stationary applications that reaches the same high efficiency (43 %) as a comparable Diesel engine, while at the same time lowering the NO_x emissions to 16 mg/Nm³ (as compared to 2400 mg/Nm³ for the Diesel).

At temperatures near 2000 K the reaction proceeds. Solar radiation is thereby directly converted into chemical energy of the form Zn and O₂. [9] To avoid the recombination, the gaseous products can be separated high temperature membrane processes or quenched. The separation step is a critical area of research. The stored solar energy in the condensed Zn phase may be used as the fuel in a fuel cell or battery. When H₂ is desired, it has also been suggested that the Zn be used to split water in an exothermic reaction. In either scenario, the ZnO is recycled to the solar furnace.

By adding carbon in some form to the system, the decomposition temperature is reduced, thereby easing the technical burden of creating the solar thermal chemical reactor. Furthermore, substituting solar process heat for the heat produced by the combustion of fossil fuels, one can reduce the Zn industry's CO₂ emissions by a factor of 10. [16] It is expected that it will be cheaper to avoid CO₂ with solar chemistry technology rather than to produce it, capture it, transport it, and store it deep in the ocean or in caverns.

Combustion processes evolve on the basis of complex interactions between fluid dynamic and chemical mechanisms, each extending over time and space scales some order of magnitudes apart from each other [18]. In addition, chemical reactions of relevance refer to both homogeneous and increasingly heterogeneous phenomena (see for example catalytically supported combustion [19], soot oxidation, solid fuel combustion etc.). This adds to the system complexity and, together with the need to understand reaction paths in oxidation of new fuels, shifts research priorities in combustion continuously towards chemistry fundamentals and chemical engineering in general.

In this context, advances in combustion science rely upon non-intrusive diagnostic techniques [20] (laser spectroscopy to investigate molecular dynamics down to femtosecond scales [21]) and direct (or as model-free as possible) numerical simulation of flames in laminar and turbulent flow fields [22]. An issue of crucial importance in combustion research is of course the cross-

fertilization of experimental and simulation methods both in enhancing and validating fundamental understanding and in development of improved combustion systems.

2.2.2. Fuel cells

Fuel cells convert chemical enthalpy into electric power via low-temperature electrocatalytic processes. The achievable efficiencies are very high, as there are no Carnot limitations as in thermal energy conversion processes. As low temperature catalytic devices, fuel cells are limited to using chemically pure and well defined fuels, such as hydrogen and possibly methanol. This means that efficient and highly selective fuel processing is a key issue for providing the right fuel for fuel cell power generators.

While the application of fuel cells was restricted to niche markets for more than 150 years, this technology has experienced a recent upsurge of interest, as a consequence of legislative initiatives targeting traffic emissions. The polymer electrolyte fuel cell technology is predominately pursued for this application, due to its intrinsic advantages of high specific power and power density (approximately 1000 W/kg and W/l for the fuel cell stack with H₂ as a fuel), low temperature start-up, and fast load-following behavior. Major problems to commercialization have still to be solved, over all the cost issue, but also technical issues of system simplification. At PSI, these problems are addressed in projects aiming at the development of low-cost high performance membranes [23], design of inexpensive light-weight stacks [24], and novel humidification concepts [25].

The problem of the on-board storage of an appropriate fuel will represent a key issue for the successful market introduction of fuel cells. Hydrogen as a fuel simplifies operation for this low-temperature fuel cell (<100 °C), and the first demonstration vehicles have followed that concept with compressed H₂ on-board. The fuel problem, including logistic aspects, may be exemplified by the fact that up to now automotive industries follows fuel cell vehicle development with different on-board fuels, e.g. compressed and liquefied H₂, and liquid methanol. The latter has to be reformed on-board, thus requiring the complicated interplay between a slow start-up and slow load-following reformer, including a purification step for the H₂-rich reformat (CO-problem), and the fuel cell [26]. Modeling well to wheel energy efficiencies of fuel cell driven automobiles, taking into account the advantage of the fuel cell's higher efficiency at part load, exhibit

values surpassing those of ICE driven automobiles (cf. [27], and references therein). Future demonstration projects have to verify these values under normal day-to-day operation conditions.

The direct electrochemical conversion of methanol in the fuel cell is an interesting concept, however major electrocatalytic and material problems as well as system problems (CO₂-removal) have still to be solved to reach for this technology the up-to-date development state of the H₂/reformat technology in the future.

Both low and high temperature fuel cells are considered promising for stationary energy conversion. High temperature fuel cells offer the advantage that CH₄ can be used as a fuel without any further pre-treatment. Of particular interest is the combination of the high temperature Solid Oxide Fuel Cell (1000 °C) with a gas turbine fueled by the exhaust gas of the fuel cell. Low temperature PEFC are increasingly considered for the market of decentralized co-generation (electricity and heat for private buildings). These demonstration projects derive their attractiveness from the perspective of this technology in the automotive application, projecting high volume production and thus low price.

Ultimately, price per kW-installed power delivered by the conversion system will be the decisive argument for the competition of fuel cell technology with internal combustion in all of these applications. Thereby, one has to realize that these traditional technologies still have a potential for further optimization.

2.2.3. Electrochemical Energy Storage

Electrochemical energy storage systems such as batteries and supercapacitors may be used in peak power shaving systems and electric automobiles. They will help to use electric power more efficiently and to alleviate the emission problem in heavily polluted cities. For these applications the cycle life, specific energy and specific power have to be improved (for most applications it would be advantageous to have a cycle life of more than 1000 cycles, a specific energy of 80-120 Wh/kg, a specific power between 80-500 W/kg at a cost of about 300 CHF/kWh).

Among the candidate systems, lithium batteries excel by their high power density [28]. By comparison, zinc/air batteries [29] offer the advantages of high energy density and low cost, and are hence promising for mobile applications with lower power demands. Electrochemical double layer capacitors (ultracapacitors [30]) have a considerable

potential to reach the necessary specifications for the recuperation of breaking energy in hybrid type vehicles. A strong effort in material

research and cell engineering will be necessary to reach all the goals mentioned.

2.3. Exhaust clean-up

Although in general it pays to focus on pollution prevention in the up-stream processes (fuel processing and energy conversion), most combustion processes cannot be made as clean as required by primary measures alone. Filters and catalytic converters have been developed as powerful tools for reducing the impact of emissions from stationary and mobile energy converters. For many applications, post-treatment of the flue gases is the most eco-efficient way of dealing with the problem of minimizing the total environmental impact. This is particularly true for coal combustion and waste incineration, where down-stream processes for removing acidic gas components (sulfur, halogen) and particulates have been developed.

Exhaust gas after-treatment is of increasing importance for internal combustion engines as applied in vehicle propulsion technology as well. In addition to the well established 3-way catalytic converter, new challenges arise with the clean-up of Diesel or lean burn exhaust gases. Two pathways are discernible at present: The first involves the optimization of the combustion process with respect to NO_x emissions, and the use of particulate filters. The second, highly promising approach is to suppress particle formation within highly efficient compression ignition engines, and to develop active modules for catalytic NO_x removal in the lean combustion gases [31]. Central issues in bringing such systems to application include the durability of components, the development of sensors and actuators for systems control, and the system

integration. Fundamental issues of research involve understanding of surface processes, advanced material properties and coupling of heterogeneous and homogeneous chemical and transport mechanisms.

The more the fuels are contaminated and heterogeneous to start with, the more important it is to find sustainable solutions for the ashes. This is of particular concern with the incineration of municipal solid waste (MSW) which contains about 25% of ash. Especially the fly ashes produced in the process of incineration are highly enriched with toxic volatile heavy metals. The deposition of such fly ashes in landfills poses an environmental hazard as the heavy metals will eventually leach out into the ground water. Sustainable use of waste materials for energy recovery requires that the solid incineration residues (fly ash and bottom ash) be treated such that the heterogeneous mix of materials contained in them can be separated to such a degree that recycling becomes possible. The design of processes for efficient recycling and energy recovery requires fundamental knowledge of the chemistry of solids at elevated temperature and of the processes governing evaporation and condensation of volatile heavy metals [32-34]. Ultimately, the development of these technologies aims at product cycles where no waste is involved, in line with the concept of industrial ecology with the vision of technical systems evolving to a degree of closing material loops comparable to the natural cycles of the chemical elements.

2.4. Impact analysis in the environment

Energy use always leaves its fingerprint in the ecosystem. This is the motivation of environmental research initiatives to contribute to the efforts for the advancement of an economic and sustainable energy use, with the goals

- to identify sources and sinks of gaseous and particulate emission from energy conversion processes

- to study the transport and the chemistry of these particulate and gaseous compounds in the atmosphere
- to investigate the effects of the deposited substances in the ecosystems

Besides local emissions in the surroundings of power plants and industry, one of the major sources of airborne substances are transpor-

tation activities, a spatially well distributed network. In the European Union, transportation is projected to increase strongly in the future, and therefore this issue is of high priority. The situation is particularly severe in the Alpine regions of Europe which represent a highly sensitive ecosystem, which is in addition exposed to high local stress in the few corridors where the North-South road traffic is concentrated [35,36].

It is not only that such an impact can drastically impair local regions, with all the consequences for the local population and the recreational value of this area. The fact that the Alps provide about 90 % of the freshwater of central Europe is a strong motivation for concentrating strong research resources in this region. A collapse of this sensitive environment would have enormous consequences for all of Europe.

The issues that need to be addressed in this context are:

- How will the air quality in this region, with its impact on quality of life and health, be influenced by increasing traffic?
- What is the impact of road transportation on the adjacent and the distant ecosystem (plant production, plant carbon / water regimes, biodiversity, ecosystem stability)?

In quantifying the impacts of air pollutants, a first necessary step is the mapping of air masses (atmospheric flux measurements) and tracing of airborne substances and particles from the source to the site of deposition (vegetation). Remote sensing and *in situ* methods combined with satellite, aircraft, and long-range, ground based sensor data complete the picture from small scale resolution to the regional scale [37]. Intensive field campaigns are needed to analyze the limiting factors for the dilution and production of primary and secondary pollutants. The results gained by these experiments are restricted in time and space. Specially developed models are used for temporal and spatial interpolation, thus allowing a large scale evaluation of transport, conversion, and deposition of air pollutants [38]. Furthermore, these models are used to design the optimum emission reduction strategy in order to e.g. reduce

regional ozone concentration or aerosol mass, and are an important tool for the characterization of future emission scenarios [39].

Not all emissions are harmful for people or the environment. Thus questions of the quality and quantity of the released particles and trace gases must be addressed. Therefore, besides tracing the substances from the sources to the site of deposition (sinks), the study of the air pollutant effects on the ecosystem is a key issue. A variety of modern physical, plant physiological and ecological approaches (gas exchange and ecosystem flux measurements, isotopic ratio mass spectrometry (IRMS) [40], dynamics of the biodiversity) provide the needed tools for assessing the impacts of air pollutants on the ecosystem. Thus changes in the carbon, water and nutrient relations, or shifts in the species compositions of plants communities and other organisms in the ecosystem represent specific indicators for the impacts of the various trace gas species. The development of the air quality in particular, and of its changes from the past to the present are a key issue for answering the question, what we can expect for the future regarding the effects of air pollutants on the ecosystem. This topic is assessed in a multidisciplinary research approach (e.g. using stable isotopes in combination with dendrochronology [41] and nutrient and biochemical analyses of the organic materials). Biological and glacial archives, such as tree rings, ice cores, and peat bog cores represent a valuable source of information about past climatic impacts on these materials [42]. Based on this information, it is possible to derive a set of parameters from these "archives" which will make it possible to distinguish natural impacts from anthropogenic influences. Latest experiments and analyses, which were carried out in this context, are very encouraging.

Finally this set of specific indicators is an important criterion in the evaluation about the efficiency of the improvement in the combustion chemistry and energy conversion processes.

3. Conclusions and outlook

Energy services, as related to food production, construction, space heating, lighting, provision of goods and services, and transportation, represent basic human needs. We have argued that it is not the energy use

itself that induces changes on a global level, but the associated material fluxes from and into the environment. The need to reduce these fluxes necessitates the use of renewable energies, minimization of material intensity,

and the cycling of materials in the production processes. Innovative approaches of using solar radiation, and cycling of CO₂ by biomass exploitation are direct outflows of this concept.

Efficient provision of energy services relies heavily on the availability of chemical fuels. Hence, a strong research focus should be devoted towards methods of producing clean, standardized chemical energy carriers from renewable feedstocks.

Selectivity and yield of chemical reactions are the key factors for providing renewable fuels and for their clean conversion to energy services (e.g. in transportation). Novel catalysts, unconventional reaction media such as supercritical gases, and exciting chemical engineering developments leading to process intensification will contribute towards minimizing the flows of reactants, auxiliaries, energy and waste associated with both the provision of fuel and the production of commodities.

Energy conversion process optimization on the basis of both the electrochemical and the thermochemical route relies heavily on an understanding of basic phenomena related to chemical reactions and surface phenomena. For example, a change in the electrocatalyst bringing the open circuit voltage closer to the thermodynamic maximum, would greatly enhance the efficiency of a fuel cell. Similarly, advances in the NO_x reduction in lean exhaust gases would allow engine designers to focus on minimizing the particulate emissions, thereby both raising the efficiency and lowering the detrimental health effects of particulates. As a consequence, a strong competence in key disciplines, such as electrochemistry and combustion, is a key towards leap-frogging advances in energy conversion.

Analysis of the chemical footprints of energy systems in the environment, and their impact on the biosphere, are a prerequisite to assess the relative importance of changes we need to make to the way we produce and use energy carriers. These studies are needed both on a

global level, addressing climate changes, and on a regional level to quantify the damages caused by pollutants specific ecosystems, such as the Alpine region.

In the past, energy research has been characterized by disciplinary fragmentation which has led to the formation of respective "schools" of thought. Energy research has been considered to be a domain of mechanical or electrical or chemical engineering alone. Resulting technologies have reflected their disciplinary origins and has often had disciplinary idiosyncrasies which have been limiting the potential of a technology. As an example: fuel cells research has for long time been an exclusive domain of electrochemical research. Bringing the fuel cell to the market and into application requires a combined effort of chemists, chemical engineers, electrical and mechanical engineers. Taking the development of fuel cells as a viable energy conversion device as a model, energy research will have to extend its interdisciplinary integration to enable the emergence of new solutions. The difficulties of innovations in the field of energy in general and renewable energy in particular, have in most cases not been technical, but rather economic and social acceptance.

Beyond the progress in natural science and engineering technology addressed in this essay the development and establishment of sustainable energy systems requires obviously a robust frame of social, economic and political conditions. To that end, establishing an efficient channel of communication between the backbone of energy technology fundamentals and social science aspects is a necessity of crucial importance as well. Acknowledging present and future societal needs, being aware of economic boundary conditions, and taking into account the choices of actors in society, business, and politics, are key elements for ensuring the successful penetration of the developed engineering solution.

Acknowledgements

The present article is based on strategic discussions which were held to define future research priorities of PSI's General Energy Research Department. We want to express our thanks to all coworkers within the department

for their contributions to the shaping of a common strategy. We thank R. Dones for discussing LCA issues regarding material flows and emissions.

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