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ENERGY AND ENTROPY FLUXES IN COAL GASIFICATION AND LIQUEFACTION PROCESSES

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PREFACE

In the long-term studies on energy systems performed at IIASA, scenarios that provide for substitutes for fossil oil and gas are considered. In the future coal is expected to contribute to energy supplies to a greatly increasing extent only if it is converted to liquid or gaseous fuels or electricity. Coal conversion systems are rather complex, not only internally but also with respect to their exchanges with the environment; some use auxiliary energy, others yield byproducts. Therefore, the evaluation of such systems is not a simple task and the comparison of very different systems – different in the nature of inputs and outputs – must not be reduced to a comparison of energy efficiencies.

Moreover, because these studies cover a long time period, it is necessary to estimate the potential development of related processes in order to determine the inputs required for producing substitute fuels. There are physical and chemical limitations to potential improvement. This paper outlines these constraints and provides means for the evaluation and comparison of different fuel synthesis processes, especially regarding methanol. The possibility of adding energy from nuclear or solar primary energy sources to such processes is discussed and the advantages are assessed.

CONTENTS

BASIC ANALYSIS

Coal, being the largest fossil energy resource, plays an important role in all future energy supply scenarios. In a solid state it cannot be used to a greatly increasing extent as a fuel for the final consumer. If converted to liquid and gaseous fuels or to electricity it is more suitable. Electricity generation from coal is very important in this context; however, this is the state of the art and it is therefore not considered in more detail in this paper. In generating electricity from coal there are constraints, for economic reasons at least, resulting from the location of coal resources and from the relatively high transportation costs for coal and electricity. Liquid and gaseous fuels produced from coal, however, could well serve as substitutes for fossil oil and gas when the latter fuels become scarce. The substitute fuels could be produced almost free of sulfur.

Gasification and liquefaction of coal have already been carried out. The principal processes used commercially are those of Lurgi, Winkler, and Koppers-Totzek for gasification, and that of Fischer-Tropsch for liquefaction. These and similar processes are being developed to improve their economy and efficiency. Furthermore, the possibility of adding external energy from nuclear reactors or solar collectors to such processes is being investigated. The advantages of the latter procedure over the autothermal coal conversion procedure (i.e., no energy other than that of coal is supplied to the process) should be greater fuel yields from a given amount of coal, decreased carbon dioxide emissions, and also possibly certain economic benefits.

Scenarios of world energy supplies in, for example, 50 years, take into account that several terawatts (TW) of methanol will have to be produced from coal and nuclear or solar energy (Haefele and Sassin 1977); it is, therefore, essential to search for efficient and economic processes for methanol production. In this study, the natural limits of these processes are evaluated against a background of the relevant thermodynamic and chemical laws. This allows a judgment to be made about the "quality" of a process and the limits to its further development. Several proposed processes, especially molten-iron bath gasification (being developed by Humboldt-Wedag in the FRG), are examined, particularly in relation to the coal and additional energy they require.

The processes for fuel production from coal have to be considered, among others, from three specific aspects: energetic, exergetic, and chemical. It is energy that is usually considered in the evaluation of fuel production processes. The energy efficiency η (i.e., the energetic value of the yield over the energetic value of the expense) is used to characterize a process. The energy efficiencies of current autothermal gasification and liquefaction processes range from approximately 0.4 to 0.75 (i.e., this fraction of the chemical energy of coal is to be found in the products, or the energy expense – coal – is 1.3 to 2.5 times greater than the energy yield).

In general, energy efficiency $\eta = 1$ is not the natural limit. Therefore, it is not sufficient to estimate the potential improvement of a process on the basis of its energy efficiency alone (Voigt 1978). Rather, such an estimate has to be made by taking into account the entropy flows that a system exchanges with its environment. This enables the entropy production, which is the absolute measure of the system's thermodynamic quality, to be calculated. Certainly, entropy is not as easily visualized in combination with energy and is not as easily handled by non-specialists. Therefore, quantitative considerations are given preferably in terms of exergy, which is defined as

$$\text{Exergy} = E - T_0 S \tag{1}$$

Exergy can be interpreted as the maximum work that can be provided by energy E that is accompanied by entropy S, if it is possible to exchange heat with an environment of temperature T_0. Exergy has the same dimension and order of magnitude as energy, it is a measure of the "quality" of energy. The ratio of exergy yield to exergy expense of a system or process is called reversibility ϵ (or exergy efficiency or second law efficiency); ϵ represents the proximity of a process to the thermodynamic limit: $\epsilon = 1$ for an ideal, reversible process; $\epsilon < 1$ for a real, irreversible process. The degree of reversibility indicates the potential for improvement of a system. The formalism for this evaluation is well known in technical thermodynamics and a single general description is given in Voigt (1978). For current autothermal gasification and liquefaction processes, the reversibility ranges between 0.35 and 0.65 (i.e., this fraction of the exergy of the coal used is found in the gas and the liquid products).

From the chemical aspect, the number of carbon atoms that are contained in a fuel are taken into account. Fossil coal can be characterized approximately in relation to its energetically relevant constituents, by the formula CH_y, with y ranging between 0.5 and 1. Between 80 and 90 percent of the exergy of coal can be attributed to carbon. Methane, methanol, and gasoline contain 0.48, 0.56, and 0.60 units of carbon, respectively (in terms of the exergy of the oxidation of carbon to carbon dioxide), in 1 exergy unit of fuel (see Figure 1). Hydrogen, of course, contains no carbon. Carbon monoxide, which is not so

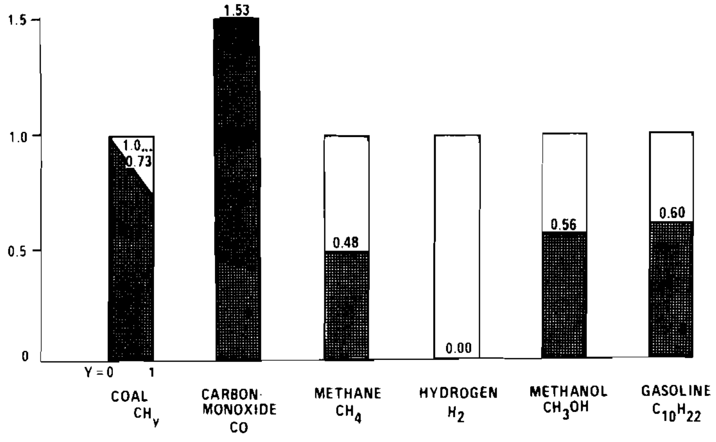

FIGURE 1 Carbon content (shaded area) of different fuels in terms of exergy.

important as fuel but essential for methanol synthesis, has less exergy than the contained carbon had in its elementary form, since one-third of the exergy has been released at the stage of carbon conversion to carbon monoxide. From Figure 1 we can see that 1.53 exergy units of carbon are "contained" in (i.e., required for) 1 exergy unit of carbon monoxide.

The figures given above represent the minimum amount of carbon necessary for the synthesis of those fuels (i.e., required for stoichiometric processes with no carbon losses). Technical processes have carbon losses, mostly in the form of carbon dioxide. The blank areas in Figure 1 indicate the minimum amount of exergy (i.e., for an ideal, reversible process) that has to be added from other sources if only the minimum carbon demand were expended. Real processes are irreversible and require a larger amount of exergy than reversible processes. Thus, the data in Figure 1 can serve as a standard against which real processes may be measured. These data may also be regarded as the asymptotic limits to further, long-term development of processes. So, it appears that the liquid fuels methanol and gasoline do not significantly differ from each other from the standpoint of carbon demand and the exergy that can be added. However, these liquid fuels differ for technical, economic, and environmental reasons and also in relation to their penetration of the market.

To evaluate real or conceivable processes, the appropriate reversible process should be used as a yardstick to measure the amount of exergy required (Voigt 1978). Consider a general fuel conversion system (see Figure 2) that is fed with coal and heat of temperature T_1 (expense), that produces a fuel (yield) – methanol in this case – and in which all other exchanges with the environment are counted as waste (dissipation). Each of these three streams (expense, yield, dissipation) is characterized by energy E, entropy S, and the number of carbon atoms N_C it contains. The conservation laws of thermodynamics and chemistry should then be applied to the processes. For

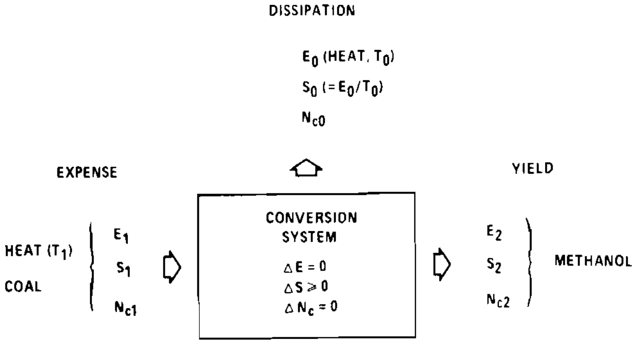

FIGURE 2 Energy (E), entropy (S), and carbon atoms (N_C) that a methanol production system exchanges with its environment.

stationary processes (all variables constant in time), using the notation given in Figure 2, these laws read:

$$E_1 = E_0 + E_2 \tag{2}$$

$$S_1 + \Delta S = S_0 + S_2 \quad \Delta S \geqslant 0 \tag{3}$$

$$N_{C1} = N_{C0} + N_{C2} \tag{4}$$

ΔS is the entropy production of the system and is not negative for the second law of thermodynamics; since energy and carbon atoms are neither produced nor annihilated, $\Delta E = 0$, $\Delta N_C = 0$. We assume that $N_{C0} = 0$, that no carbon atoms are wasted, and that $E_0 = T_0 S_0$, all wasted energy is heat of environmental temperature T_0. Then, taking into account the thermodynamic properties of carbon and methanol, we arrive at a relation between E_1 and E_2 that depends on T_1 (temperature of expended heat) and on ΔS (entropy production of the system). In Figure 3, the energy expense E_1 is plotted (left-hand scale) against the temperature T_1 and normalized for the yield of 1 energy unit of methanol, $E_2 = 1$. Of the total energy expense, 0.54 units are expended as coal (if it were devoid of hydrogen), the remainder is heat. The curve $\epsilon = 1$ is valid for reversible processes, $\Delta S = 0$. For example, if heat of 800 Kelvin (K) is available, 0.68 units of heat have to be added to the 0.54 energy units of carbon, resulting in a total energy expense of 1.22 units for 1 energy unit of methanol; therefore, 0.22 units of energy are inevitably wasted. This is the absolute minimum dissipation of energy and serves as the yardstick for real, irreversible processes. The corresponding energy efficiency η (0.82 in this case) can be read from the right-hand scale.

For a lower degree of reversibility, for example, $\epsilon = 0.5$, if the coal expense is held at the chemical minimum (0.54), the expense of heat required is more than doubled and increases to 2.2 units of 800 K heat. So, the total

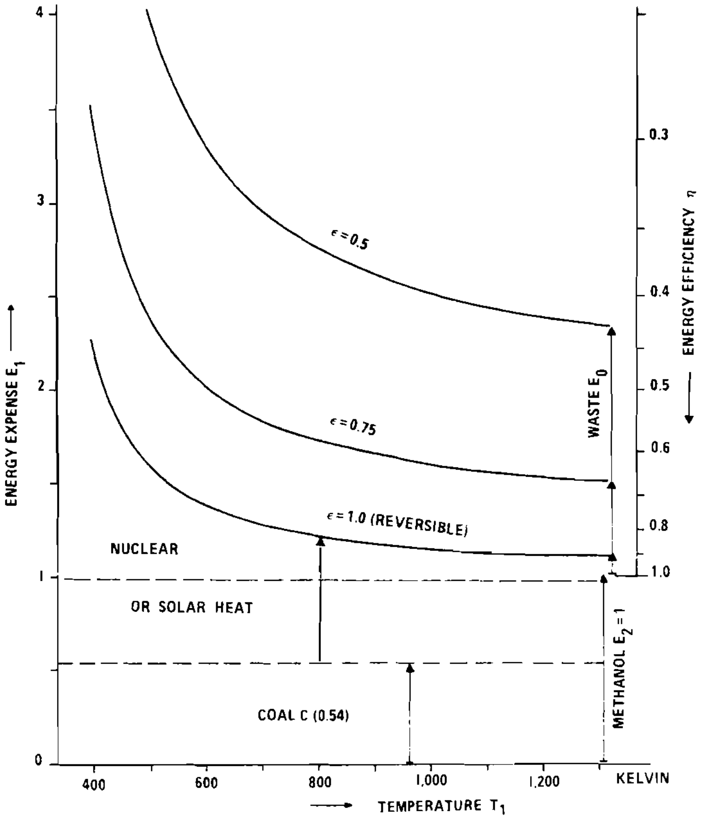

FIGURE 3 Energy expense E_1 (heat + coal) required to produce 1 unit of methanol for reversible ($\epsilon = 1$) and irreversible ($\epsilon < 1$) processes.

energy expense is 2.8 units for 1 unit of methanol, 1.8 units being wasted (see curve $\epsilon = 0.5$ in Figure 3).

THE REFERENCE CASE

Figure 3 illustrates how real or proposed methanol production processes with a known coal and heat input can be evaluated to determine how "good" the processes are (i.e., how far they are from natural limits). To proceed further, we take into account some more practical conditions, and, by making plausible assumptions about the main subsystems, arrive at an estimate of the energy efficiency that could be attained in the future. This is dependent on several factors.

Given certain technologies, in many cases reversibility can be improved by extending the equipment (e.g., enlarging the heat transfer area or using an expansion turbine instead of a throttle valve), which usually implies increasing capital investment. Therefore, the design of capital-intensive thermodynamic

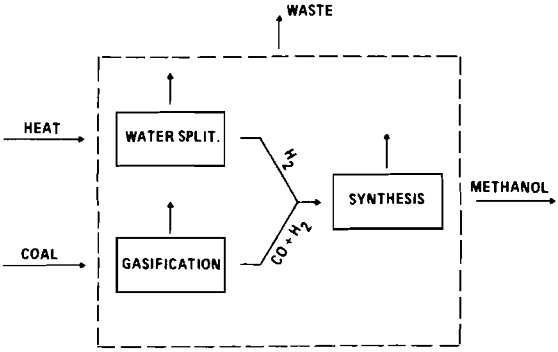

FIGURE 4 Main subsystems for methanol production from heat and coal.

equipment (e.g., thermal power plants) is made after carefully balancing the capital cost against the resulting increase in the product's value. A formalism for such an optimization procedure is given in El-Sayed and Evans (1968). With a long-term perspective, however, technological conditions cannot be considered as fixed. Through research and development, new ideas, new processes, and new materials are produced, all of which increase the efficiency and simultaneously decrease the extension and cost of equipment. The evolution of steam engines (both piston-engines and turbines) provides a good example of this. Therefore, for our estimate of reversibility, the basic thermodynamic and chemical principles, but not the technological or economic conditions, are regarded as fixed. As a consequence, the subsystems of the fuel conversion processes considered are characterized primarily by their task or function, rather than by fixed techniques.

In present coal gasification plants, hydrogen requirements are covered by carbon monoxide shifting. Since this is coupled to carbon dioxide production (i.e., wastage of carbon atoms), which should eventually be avoided, additional hydrogen production that is independent of carbon has to be provided. Therefore, the main subsystems for methanol production considered are gasification (including carbon monoxide shifting if it exists), water splitting, and synthesis (see Figure 4).

To achieve ideal conditions for gasification processes – no wastage of carbon, $N_{C_0} = 0$, and, simultaneously, no entropy production, $\Delta S = 0$ – it would be necessary to take up entropy (together with heat) from the environment, $E_0 < 0$, therefore, $\eta > 1$. This is because of the entropy balance in which the entropy of one mole of the products is larger than that of the inputs. It is unlikely that this will become technically feasible, because a type of reversible heat pump would have to be included in the system. Therefore, instead of taking $\Delta S = 0$ for the reference case, we prefer to take $E_0 = 0$, where no energy is wasted (i.e., $\eta = 1$). Thus, the reversibility is approximately 0.9, which is still a satisfactory figure. Besides carbon, which has already been

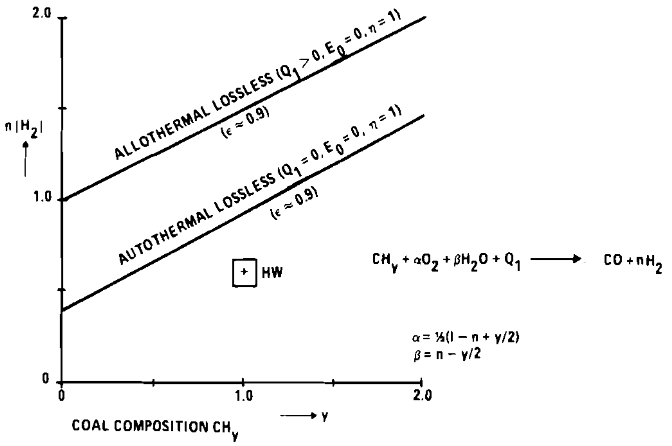

FIGURE 5 Hydrogen content n of synthesis gas, $CO + nH_2$, as a function of coal composition CH_y, for lossless ($E_0 = 0$, $\eta = 1$) autothermal ($Q_1 = 0$) and allothermal ($Q_1 > 0$) gasification (HW: Humboldt-Wedag gasification).

considered, the only other element of coal having major energetic and exergetic relevance is hydrogen. The hydrogen content ranges from 0.5 to 1 atom of hydrogen per atom of carbon; brown coal and lignites have on average 0.95 and pit coal and anthracites have 0.7 (Nesterov and Salmanov 1977). The essential feature of coal is that, relative to the energy of oxidation, hydrogen is bound very loosely to the carbon. In gasification processes producing synthesis gas for methanol synthesis, it is desirable to obtain a gas with a large hydrogen content, since this provides hydrogen that would otherwise have to be generated in other ways.

In Figure 5 the composition of synthesis gas, $CO + nH_2$, for two types of gasification processes is plotted against the hydrogen content of the coal used, y, according to the formula CH_y. The lower line represents autothermal processes (i.e., no energy other than that of the coal is supplied to the gasification process, $Q_1 = 0$) that are "lossless," $E_0 = 0$ (i.e., no energy is dissipated). The energy efficiency for the gasification subsystem, therefore, is $\eta = 1$, and the reversibility is $\epsilon \approx 0.9$. The hydrogen content of the product gas ranges from $n = 0.4$ molecules for pure carbon input to $n = 0.95$ molecules for coal input of composition CH. Allothermal processes (i.e., extraneous heat is added to the process, $Q_1 > 0$, see Figure 5, upper line) permit larger amounts of water to be added. If carried out without energy losses, $E_0 = 0, \eta = 1$, these processes yield a maximum of $n = 1$ to 1.5 hydrogen molecules for coal of composition C and CH ($y = 0$ and $y = 1$), respectively. For methanol synthesis, the hydrogen demand is $n = 2$ molecules of hydrogen; therefore, if coal with a large hydrogen content is used, only one-half of a hydrogen molecule has to be provided from other sources. Figure 5 extends to $y = 2$ (i.e., CH_2 as source composition). CH_2 no longer represents coal but mineral oil, and corresponds approximately to the present method of methanol production. However, the use of oil is exactly what should be avoided in the future. The composition of the gas for the molten-iron bath gasification process, to be dealt with later, is indicated by the cross (HW) in Figure 5.

For the water-splitting subsystems (see Figure 4), if electricity is expended, the technically attainable reversibility is estimated to be approximately $\epsilon = 0.75$, which corresponds to an energy efficiency of $\eta = 0.9$ (Getoff 1977). The conversion of heat to electricity in large thermal power plants is carried out today with an energy efficiency of $\eta = 0.40$ for $T_1 = 800\,\mathrm{K}$ and $\eta = 0.32$ for $T_1 = 600\,\mathrm{K}$; this corresponds to a reversibility of $\epsilon = 0.64$ in both cases. Although improvements in thermal power plants are also to be expected in the future, for the moment we shall retain these figures; the influence of an improvement is discussed later. Therefore, for the total water-splitting subsystem, starting with heat, we take an overall reversibility of $\epsilon = 0.5$ as the reference case. This could also be valid for thermochemical water-splitting processes developed in the future.

The synthesis of methanol from synthesis gas represents the state of the art. We take as the reference case a situation where no matter is lost, where the energy and the exergy differences between the (cold) synthesis gas and the liquid methanol are lost but no auxiliary energy is supplied. This gives a reversibility of $\epsilon = 0.96$, which is a very satisfactory figure, and an energy efficiency of $\eta = 0.85$.

For the reference case (see Figure 6), the total energy expense (upper line) and the shares of coal and heat are plotted against the hydrogen content y of the coal used. These lines are valid for lossless autothermal gasification, given heat of temperature 800 K. The importance of hydrogen in coal becomes obvious from a glance at Figure 6. For the case of coal of composition C (e.g., coke), there must be an expense of 0.54 energy units of this coal plus 1.75 units of heat, making a total of 2.3 units for the production of one energy unit of methanol or an energy efficiency of $\eta = 0.43$. In this case, the reversibility, given in Figure 3, is $\epsilon \approx 0.6$. For hydrogen-rich coal, e.g., coal of composition CH, 0.75 energy units of this coal plus 1.2 units of heat are necessary, giving an overall efficiency of $\eta = 0.52$ and a reversibility of $\epsilon = 0.66$.

Figure 6 also includes figures related to the molten-iron bath gasification process (from a private communication with R. Pfeiffer, KHD Industrieanlagen AG, Humboldt-Wedag). In this process, which is similar to steel-making processes, oxygen and steam are blown into a bath of molten iron and dissolved carbon at a temperature of approximately 1,600 K. Under such conditions, the gases react with the carbon to form carbon monoxide and hydrogen, and the generation of carbon dioxide can be avoided. The carbon extracted during the bath process is replaced continuously by granulated coal, which is also blown into the bath. All types of coal are considered to be suitable. During the process, the sulfur content of the coal combines with and is thus removed with the slag, and one can expect that almost

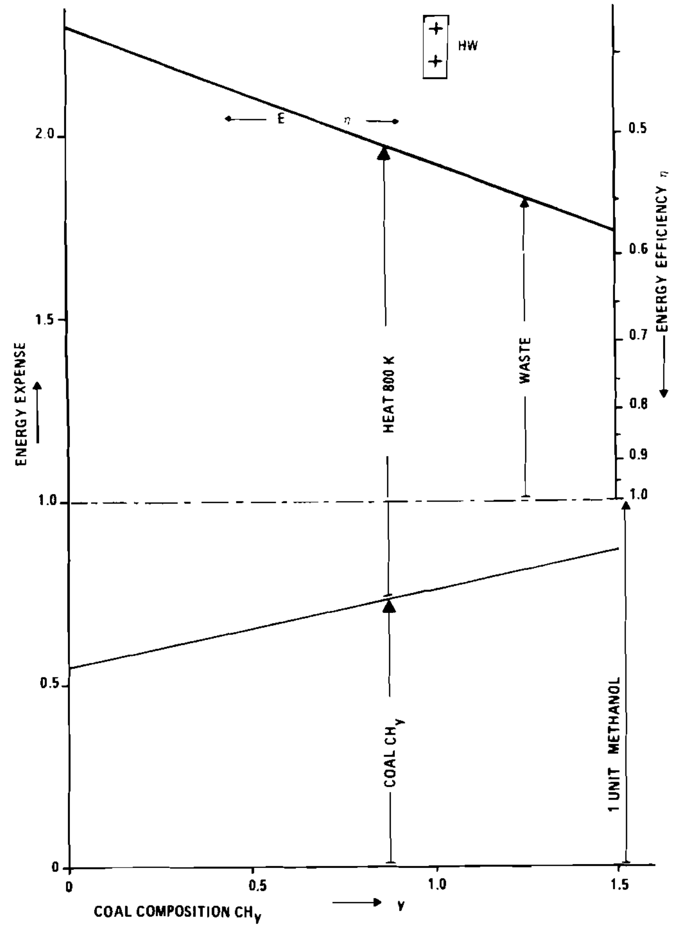

FIGURE 6 Energy expense (800 K heat + coal) required to produce 1 unit of methanol, as a function of coal composition CH$_y$, for lossless autothermal (upper line) and Humboldt-Wedag gasification (HW).

no carbon will be lost. The energy lost as heat from the bath is small compared to the large energetic throughput (about 10^7 W/m^2 of molten-iron bath) which is 30 times the black radiation at 1,600 K. The only difficulty, with respect to energy, is that the product gases (and slag) are emitted at that high temperature, taking with them about 12 percent of the energetic throughput as sensible heat. If, under ideal conditions, all this sensible heat could be fed back to the process (for preheating the input), we would arrive at the lossless autothermal process already considered (upper line in Figure 6, lower line in Figure 5). If, however, under the worst conditions, all the sensible heat is dissipated, this energy must be provided by the gasification reaction, which then has to be made exo-

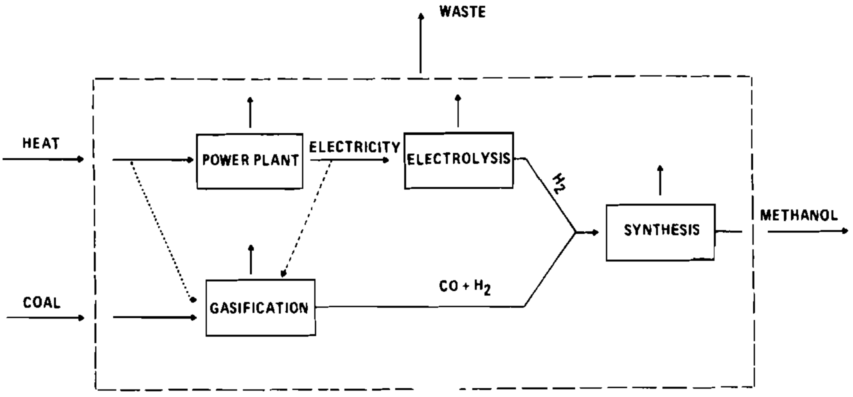

FIGURE 7 Configurations for methanol production using allothermal gasification.

thermally. As a consequence, less steam can be applied and hence less hydrogen can be produced (indicated by the cross (HW) in Figure 5). Since the hydrogen production is lower, extra hydrogen must be produced in other ways and thus additional auxiliary energy – heat of temperature 800 K – is required (indicated by the upper cross (HW) in Figure 6). As a compromise, one could consider transforming the sensible heat of the effluent gases into electricity with an energy efficiency of $\eta = 0.4$, corresponding to a reversibility of $\epsilon = 0.65$ (indicated by the lower cross (HW) in Figure 6).

The considerations above indicate the importance of carrying out the gasification process as far as possible without losses. For allothermal processes, in which external heat is added, not only is it possible for heat losses to be reimbursed but also more water can be fed into the gasification process. Thus, the hydrogen content of the product gas can be raised considerably (see the upper line in Figure 5). The additional heat can be used directly and completely to "split" water. This heat has to be provided at the temperature of the molten-iron bath, 1,600 K, and has to be introduced into the bath at a considerable power density, 3 to 5 MW/m^2 of molten-iron bath. In the near future it does not seem likely that nuclear or solar heat will fulfill this requirement directly. Nevertheless, such a possibility is indicated by the dotted line in Figure 7 and the resulting large saving in energy (lossless allothermal gasification) is visible in Figure 8, where the dotted line represents the total energy expense. The upper section beneath this line shows the fraction of 1.600 K heat, the middle section indicates the amount of 800 K heat (for electrolysis), and the base section gives the coal requirement. For the example coal of composition CH ($y = 1$), it is necessary to add only 0.77 units of heat (0.54 units at 800 K and 0.23 units at 1,600 K) to the 0.75 units of coal of composition CH, where 0.75 represents the chemical minimum. The overall energy efficiency, therefore, is $\eta = 0.66$.

This saving in energy, resulting from the energetically "cheap" production of hydrogen through the admission of heat of temperature 1,600 K into the

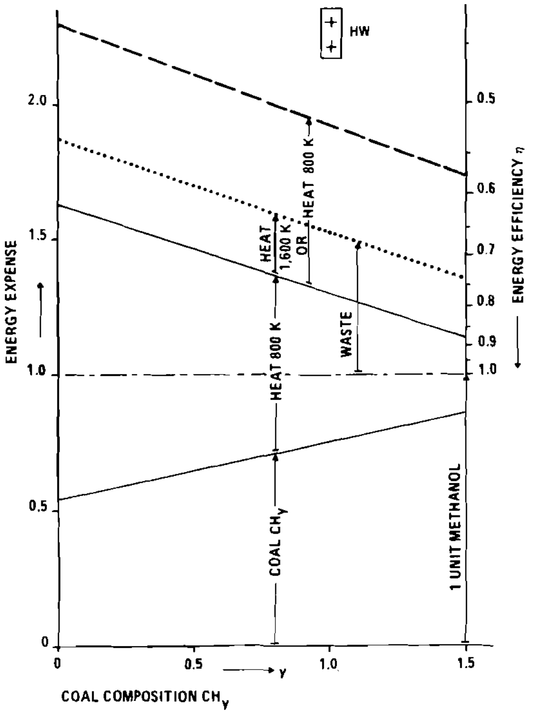

FIGURE 8 Energy expense (800 and 1,600 K heat and coal) required to produce 1 unit of methanol, as a function of coal composition CH_y, for lossless allothermal gasification. HW: Humboldt-Wedag gasification, $\cdots\cdots$ 800 K heat + 1,600 K heat + coal, - - - - 800 K heat + coal.

gasification process is desirable. Since there seems to be no possibility, at present, that this heat could be provided directly by nuclear or solar energy, it might be suitable to introduce a type of "heat pump" into the process. Certainly no heat pumps in the conventional sense exist for such high temperatures. However, *the combination of a thermal power plant (supplied with heat of temperature T_1 and dissipating heat at T_0) and electrical heating at temperature T_2, with $T_1 < T_2$, is indeed a form of heat pump*, although not a reversible one. At present, for $T_1 = 800$ K, the efficiency of electricity generation is 0.4, and the efficiency of electrical heating can be taken as $\eta = 0.9$ at 1,600 K (inductive, arc, or resistive heating), therefore the overall energy efficiency of such a heat pump is $\eta = 0.36$. This corresponds to a reversibility of $\epsilon = 0.47$, which is a reasonable figure and comparable to that of conventional heat pumps and cooling equipment. The figure $\epsilon = 0.47$ is based on the energy efficiency of a reversible process, which is supplied with heat of temperature $T_1 = 800$ K, yields heat of temperature $T_2 = 1{,}600$ K, and dissipates heat at $T_0 = 300$ K, thus $\eta_{rev} = [(800 - 300)/800][1{,}600/(1{,}600 - 300)] = 0.77$. Such a means

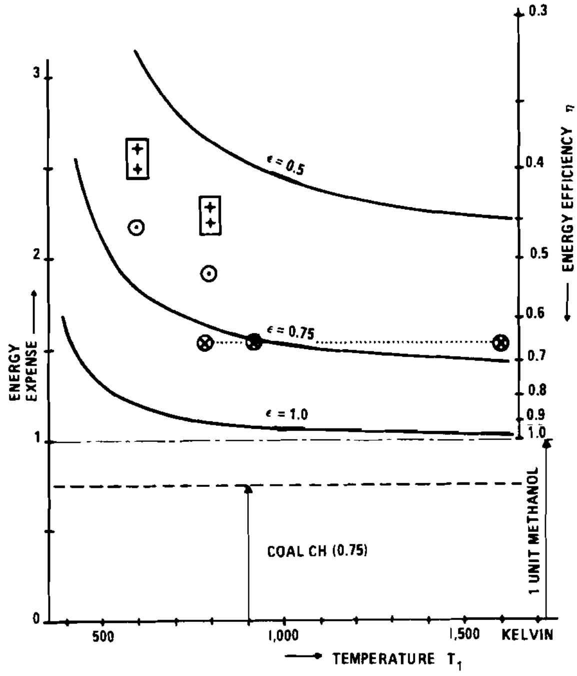

FIGURE 9 Energy expense for 1 unit of methanol for reversible ($\epsilon = 1$) and irreversible ($\epsilon < 1$) processes. ⊞, Humboldt-Wedag + power plant ($\epsilon = 0.64$) + electrolysis ($\epsilon = 0.75$); ⊙, Lossless autothermal + power plant ($\epsilon = 0.64$) + electrolysis ($\epsilon = 0.75$) or lossless allothermal (electr. heated, $\eta = 0.9$) + power plant ($\epsilon = 0.64$) + electrolysis ($\epsilon = 0.75$); ⊗, Lossless allothermal (high temp. heat) + power plant ($\epsilon = 0.64$) + electrolysis ($\epsilon = 0.75$).

of providing 1,600 K secondary heat from 800 K primary heat is indicated by the broken line in Figure 7, and the total energy expense is represented by the broken line in Figure 8 (for varying compositions of coal). This energy expense, however, amounts to the same as for the autothermal process, hydrogen being electrolytically produced to compensate for the hydrogen lacking in the synthesis gas (Figure 6). Thus, the overall result for the allothermal and autothermal processes is the same. This result must not be regarded as negative. It indicates that the choice between the two processes is not restricted by energetic considerations since in this respect the processes are comparable, but it can instead be based on technical and economic factors.

The reversibility for these examples is shown in Figure 9, where again the energy expense is plotted against the temperature T_1 of the heat expended in the case of coal of composition CH ($y = 1$). Curves of constant reversibility ϵ are given. Detailed energy and exergy flows, energy efficiency η, and reversibility ϵ for the main subsystems are put together in Figure 10 for the configuration proposed as the reference case. For gasification and electrolysis, the

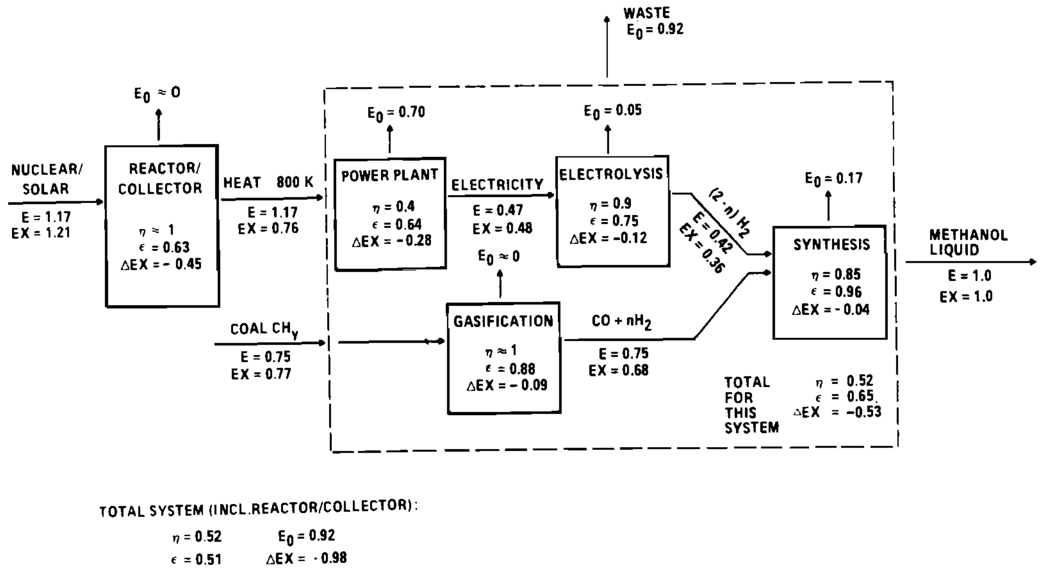

FIGURE 10 Energy (E) and exergy (EX) flows in a methanol production plant (reference case).

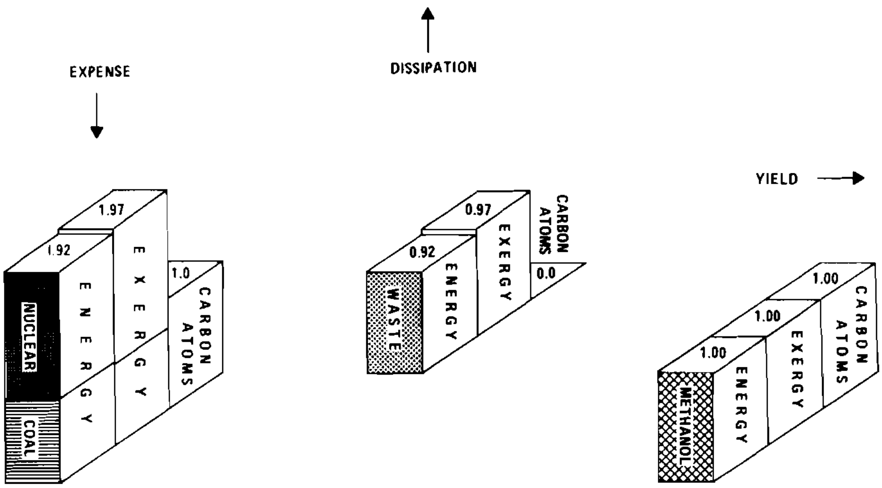

FIGURE 11 The expense of energy, exergy, and carbon atoms required for the production of 1 unit (respectively) of methanol from coal and nuclear energy (reference case).

figures are optimistic but not unrealistic; however, those for the power plant and the synthesis process are conservative.

For the sake of completeness, the production of the expended heat is taken into consideration (Figure 10, left-hand side). For simplicity, the energy efficiency is taken to be $\eta = 1$ for producing the heat by means of a nuclear reactor or a solar collector (for a nuclear reactor and for a concentrating mirror system, this assumption is almost valid). In the reference case, $T_1 = 800$ K, the reversibility for this heat production from primary high quality energy is $\epsilon = 0.63$.

With regard to the expense of primary energy – coal of composition CH and nuclear or solar energy – the total methanol production plant has overall energy and exergy efficiencies of about 0.5. By itself this result is not exciting, but when considered in conjunction with the fact that only the minimum of carbon atoms are used, it appears a relatively attractive means of producing a substitute for fossil oil. Over the long term, improvements in electricity generation are to be expected until methanol is produced on a large scale. To speculate (we will not argue about details), either the temperature could be raised considerably (high temperature reactor) or the reversibility of the thermal conversion process could be improved. Here, only the consequences of such an improvement should be mentioned (e.g., a rise in the energy efficiency from $\eta = 0.4$, as in the reference case, to $\eta = 0.5$). The total energy efficiency η would then increase from 0.52 to 0.59, and the reversibility ϵ from 0.51 to 0.58. The entire lossless and reversible electricity generation from nuclear or solar energy would raise both sets of figures to about 0.8.

So, the reference case, as outlined in Figure 10, can be regarded as a real-

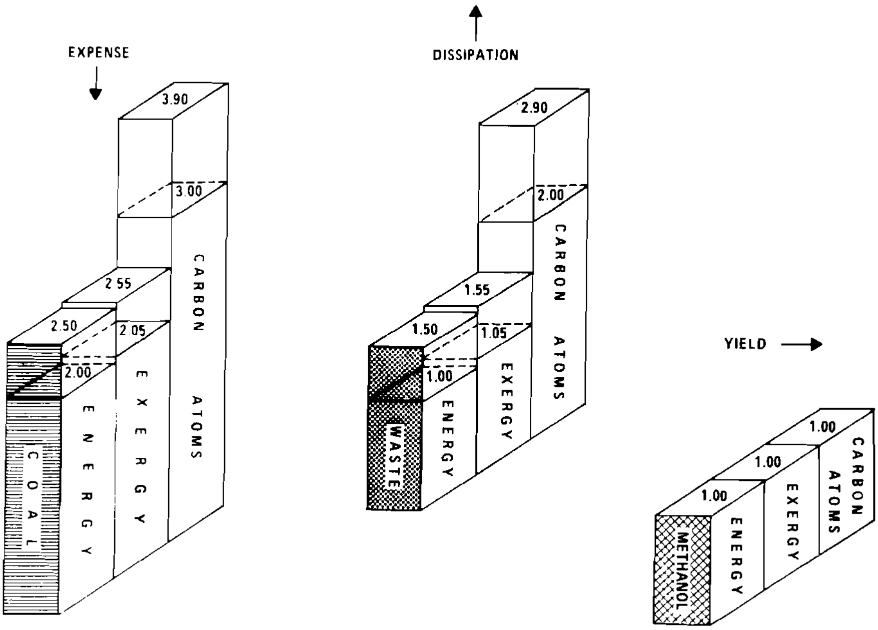

FIGURE 12 The expense of energy, exergy, and carbon atoms required for the production of 1 unit (respectively) of methanol from coal alone (two estimates).

istic technical yardstick by which proposed processes and the development of present processes can be measured. The hypothetical, fully reversible process, $\epsilon = 1$ (the requirements of which have been given in Figure 1), remains the ultima ratio.

The expense, dissipation, and yield of energy and exergy and carbon atoms are represented in a simplified form in Figure 11 for the reference case, normalized for yield = 1 for each of these quantities. It should be emphasized that the reference case includes optimistic assumptions about the gasification and hydrogen-generating subsystems that have not yet been proved to be attainable for large-scale technical equipment.

COMPARISON OF ALTERNATIVES

It is beyond the scope of this investigation to collect all attainable data of processes relevant to methanol production that are under development or consideration and to measure the more technically- and economically-based estimates against the reference case given here. Nevertheless, this should eventually be done. In one of the studies being undertaken at IIASA the technical and economic feasibility of using molten-iron bath coal gasification with additional electrolytic hydrogen for methanol synthesis is being examined and will be reported separately. Our reference case has been chosen with special regard to this system.

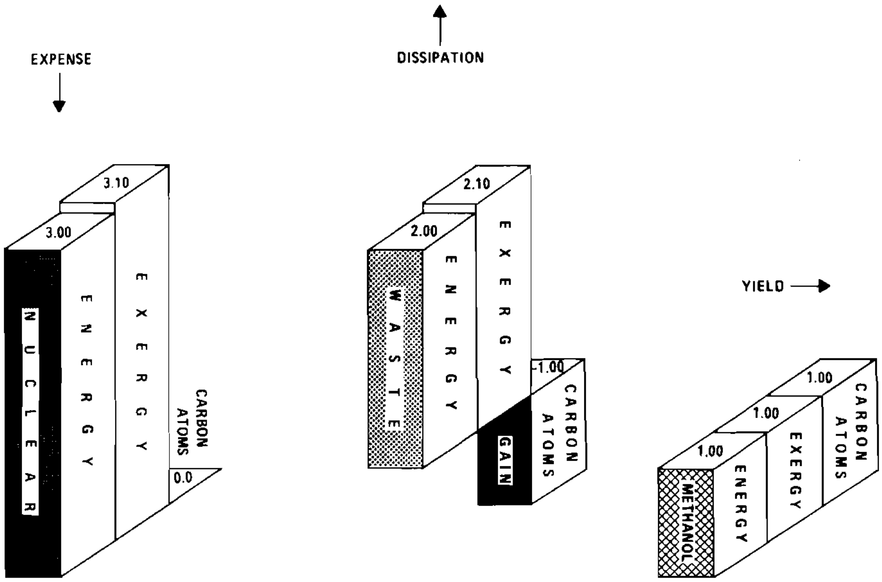

FIGURE 13 The expense of energy, exergy, and carbon atoms required for the production of 1 unit (respectively) of methanol from nuclear energy alone.

At this point two extreme examples of methanol production should be mentioned: methanol produced solely from coal and methanol produced solely from nuclear energy.

In the case where coal is used as the sole source of energy (and of carbon atoms) for methanol production, two governmental studies (Ministry for Research and Technology 1974 and Oversight Hearings 1975) estimate an expense of 2 to 2.5 energy or exergy units of coal for the production of 1 unit of methanol. Waste energy is, therefore, 1 to 1.5 units, and the energy efficiency is 0.5 to 0.4, respectively. However, 2 to 3 carbon atoms have to be dissipated (as carbon dioxide) to gain 1 carbon atom in a methanol molecule (see Figure 12).

In the other extreme case, where nuclear energy is used as the sole energy source, the possibility of extracting carbon dioxide from the air or seawater is considered. Under ideal conditions, the energy expended in separating carbon dioxide from the air amounts to less than 3 percent of the chemical energy of methanol. Therefore, it is not important whether the separation is carried out with a high degree of energy efficiency. The main problem is the considerable size and cost of the facilities required for the separation. Most of the energy expense, however, is necessary for the production of hydrogen since in this case 3 molecules of hydrogen are required for methanol synthesis:

$$CO_2 + 3H_2 = CH_3OH + H_2O \qquad (5)$$

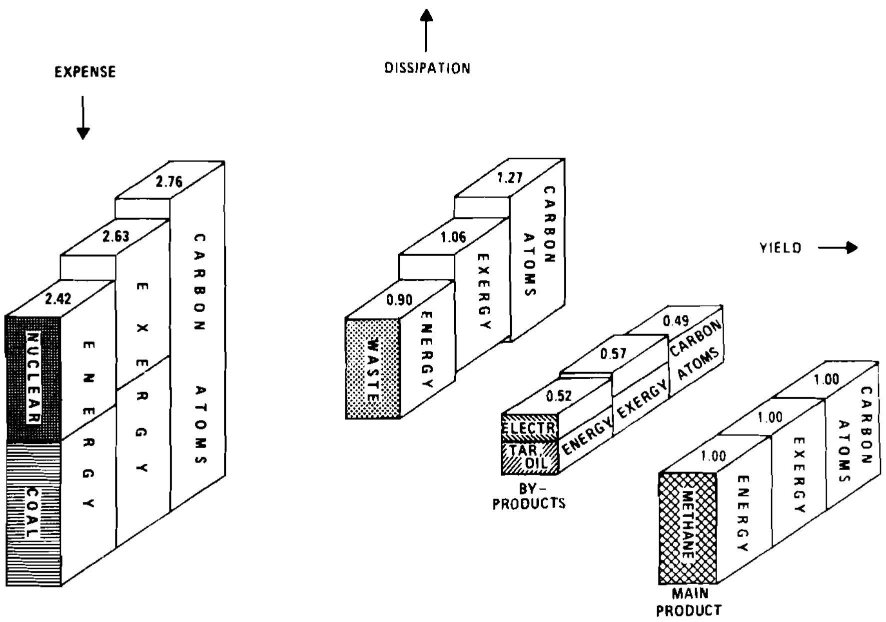

FIGURE 14 The expense of energy, exergy, and carbon atoms required for the production of 1 unit (respectively) of methane from coal and high temperature reactor heat. Source: Nuclear Research Installation (1977).

Estimates of technically feasible processes for producing methanol in this way, therefore, depend strongly on the efficiency of hydrogen production. Overall efficiency rates of between 58 and 94 percent, based on the electrical energy expense, can be expected (Steinberg and Baron 1977). An electrolysis efficiency of 0.9 (a reversibility of 0.75), as in the reference case, would result in an efficiency rate of 83 percent for methanol, based on electrical energy expense. Together with the reference case figure of $\eta = 0.4$ for electricity generation from 800 K heat or from nuclear energy (if this is converted with $\eta = 1$ to heat), we arrive at an overall efficiency of 0.33 for methanol produced from nuclear energy alone. Therefore, from the viewpoint of coal resources and carbon dioxide release, in this attractive option 2 units of heat are dissipated for the production of 1 unit of methanol, but no fossil carbon is used or wasted (see Figure 13). To be more exact, -1 atom of carbon is dissipated (i.e., 1 atom is gained, since it is withdrawn from the air or seawater).

To our knowledge there is only one project at an advanced stage that adds heat from a nuclear source to a gasification process: the "Project Prototypanlage Nukleare Prozesswärme (PNP)", led by an association of German industries and institutions. From 1975 to 1976 basic concepts for different coal gasification processes using heat from nuclear sources (a high temperature reactor) were developed for large-scale plants (Nuclear Research Installation 1977). One of these processes, steam gasification for the production of methane, is represented by its gross balance in Figure 14. For the production of 1 unit of the principal product, methane, about 0.5 to 0.6 units of energy, exergy, or carbon appear in the by-products – electricity, tar, and oil; 0.9 to 1.3 are dissipated in the environment; therefore an expense of 2.4 to 2.8 units of energy, exergy, and carbon is required. Coal and nuclear energy contribute almost equal shares to the energy and exergy expense. This may not appear very satisfactory compared to the reference case, but it has to be taken into account that this project is already at an advanced stage. The detailed planning for a prototype of 750 megawatts (MW) will be completed in 1982, whereas the reference case should be considered as a long-term asymptote.

To return to the initial problem concerning the primary energy requirements for the substitution of methanol for fossil oil over the long term, the answer, in simple and summarized terms, is that:

1 TW methanol requires 0.8 TW coal + 1.2 TW nuclear
or 2 TW coal solely
or 3 TW nuclear solely.

At present, short term requirements are estimated to be 20 to 50 percent larger than those given above.

From this and other aspects such as resources, the environment, economics, market penetration, it is expected that, given our present knowledge, the coal plus nuclear option will be the most attractive, with the possibility of a smooth transition to a solely nuclear option in the future.

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