



Energy research Centre of the Netherlands

Modeling tools for the design of pre-combustion decarbonisation reactors and zero emission power plant

Cato WP 2.2 Deliverable 15

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ECN-E--09-027

May 2009

Revisions		
A		
B		
Made by: J.W. Dijkstra	Approved: R.W. van den Brink	ECN Hydrogen and Clean Fossil Fuels
Checked by: J. Boon	Issued: F.A. de Bruijn	

Acknowledgement/Preface

This report is deliverable number 15 of CATO work package 2.2, Pre-combustion decarbonisation: "Modeling tools for the design of PCDC reactors and zero emission power plants". The Dutch Ministry of Economic affairs (EZ) is gratefully acknowledged for funding of the activities in the framework of the BSIK CATO Program and ECN ES programmes. The work also uses results of the EOS CAPTECH, EDI H2MR and the EU Cachet project, for which respectively funding Dutch Ministry of Economic affairs (EZ) and of the European Commission are gratefully acknowledged.

Abstract

For the design of power plants with CO₂ capture pre-combustion decarbonisation a set of modeling tools has been developed. System assessments are being done using Aspen Plus. A two-level approach has been developed: in the first one the heat integration is done in a simplified way, and in the second level additional details and restrictions are taken into account. For simulation of novel technologies for pre-combustion decarbonisation specialized models are available. For membrane reactors a 1-dimensional model is capable of calculating the performance while accounting for concentration gradients along the membrane length coordinate. For simulation of sorption enhanced reactors a 1-dimensional dynamic model is available that gives the reactor performance and also the time and spatial description of the reaction with absorption and desorption processes.

The results of the modeling are used in a generalized plant economic model that calculates the investments and from this the cost of electricity and specific costs of CO₂ avoidance.

Keywords

CO₂ capture, pre-combustion decarbonisation, membrane reactor, sorption enhanced reactor, modeling, process modeling, economic evaluation.

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Summary

For analysis of pre-combustion decarbonisation reactors and zero emission power plants a set of modeling tools is available. These tools have been developed or adapted and used at ECN in the CATO program on development of technology for power production with CO₂ capture.

The tools are used to assess the technical and economic feasibility of reduction of the energy penalty associated with CO₂ capture. For this the thermodynamic efficiency and costs of CO₂ capture are calculated using these models. The tools used for reactor modeling also provide insights in importance of the physical and chemical phenomena present, and on the design of these reactors.

A schematic of the use of modeling tools is provided in Figure S1. The central tool is Aspen Plus. This is a flow sheeting tool in which the whole power plant is modelled thermodynamically. It uses input from literature, experiments, detailed models and a separate gas turbine simulation program (GT-PRO). Separate from this, or integrated (for membrane reactors only) there are sorbent reactor or membrane reactor models for evaluation of the performance and design of these units. The results from Aspen Plus are used in an economic model. This estimates the main dimensions of all equipment and associated investments. It also calculates the costs of electricity and costs for CO₂ avoidance. The Aspen Icarus Process Evaluator is a stand-alone programme that can be used for provide input for the economic model.

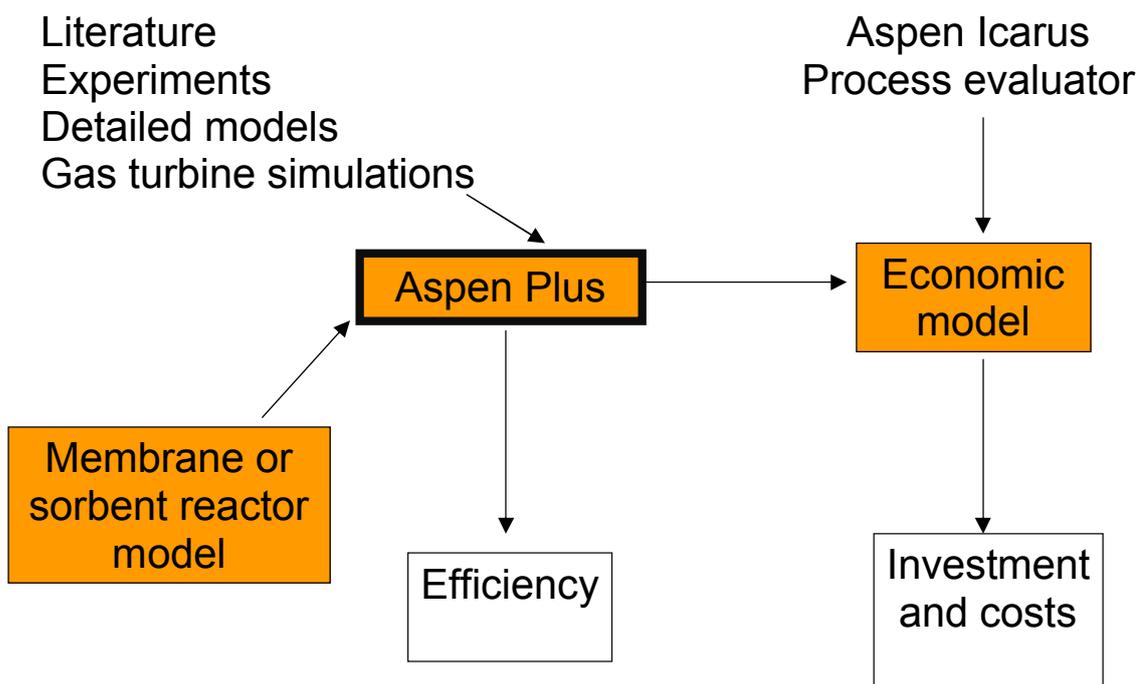


Figure S.1: Overview of modeling tools for power plants used in the CATO project.

For membrane reactors a generalized 1-dimensional model is available for calculating the performance of reformer membrane reactors and water gas shift membrane reactors. It accounts for the important effect of change of partial pressure profiles along the membrane length. The model describes all three sections of the membrane reactor, feed side, seep side and membrane accounting for chemical reaction, permeation and heat effects. Given the feed and sweep specifications and a value for the membrane surface area the model provides the outlet compositions and the partial pressure and temperature profiles along the membrane reactor length.

For sorption enhanced reactors a similar, but dynamic 1-dimensional model is available for simulation of the time dependent process. It accounts for the chemical reaction, mass and heat balance, and absorption isotherms. Given the feed and product specifications, the model calculates the profiles, for CO₂ loading of the sorbent, gas phase concentrations and temperatures along the reactor length, and as a function of time. The model can both simulate the adsorption step as well as the desorption step in the sorption enhanced reactor operation and can find the cyclic steady state that is approached in time.

For system simulations a two-step approach has been used. In the first step the systems are simulated using shortcut models (consisting of Aspen Plus standard models) and simplified heat balance calculations (using a pinch analysis approach). This provides information about the attainable system efficiency and some guidelines for sizes. In the second step detailed equipment models are used, and the heat integration is done in more detail (accounting for practical limitations for heat integration). This step provides input for detailed cost estimations.

For economic evaluation a cost model is available consisting of standard content worksheets. These contain general starting points for economic evaluations, case specific process data and investment estimation methods for various types of process equipment. Applying these sheets to all the components in the scheme, and using the data of the process simulation, the total investments for the systems are obtained. Then using cash flow time series the costs of CO₂ avoidance can be calculated using a net present value approach.

1. Introduction

1.1 General introduction

This document describes modeling tools for pre-combustion decarbonisation reactors and zero emission power plants. These tools have been developed or adapted and used at ECN in the CATO program on development of technology for power production with CO₂ capture.

Modeling can be done at various levels and with various objectives. In the CATO program models have been used for the following purposes:

- Asses the economic feasibility of power production with CO₂ capture.
- Assess the feasibility of reduction of the energy penalty associated with CO₂ capture
- Assess the sizing and construction of reactors used in power plants with CO₂ capture.
- Determine working conditions and performance targets for reactors and other equipment used in power plants with CO₂ capture.

This report focuses on the models relevant for design and evaluation of power plants with CO₂ capture. It does not treat models used for detailed evaluation and understanding of unit operations, or processes taking place therein. It focuses on those models relevant for design and evaluation only.

1.2 Pre-combustion decarbonisation with membrane reactors or sorbent reactors.

There is a growing awareness that energy must be produced at lower greenhouse gas emissions. Fossil fuels, though, will remain the most important energy source for the first half of this century. This has led to new technologies to reduce the emission of the CO₂ produced from the burning of fossil fuels. One of the options is to use pre-combustion decarbonisation. Here, the CO₂ produced is captured prior to combustion, while transferring the energy content of the fuel to hydrogen.

Various pre-combustion routes for electricity production have been investigated, using a membrane reactor or the sorption-enhanced reaction process. The general scheme of such a process is depicted in Figure 1.1. Natural gas is mixed with steam, and optionally fed to a reformer or, with additional air or oxygen, to an autothermal reformer, where it is converted into predominantly CO and H₂. The products are fed to a membrane or sorbent reactor. Here the CO and H₂ are further converted into CO₂ and more H₂. In parallel, either the H₂ (using membranes) or CO₂ (using sorbents) is separated from the stream. The H₂ is fed to a gas turbine with a heat recovery steam generator producing the power. The CO₂ is available for cleanup and compression. Instead of using the optional reformer, the conversion of CH₄ can also directly be done in the membrane or sorption reactor.

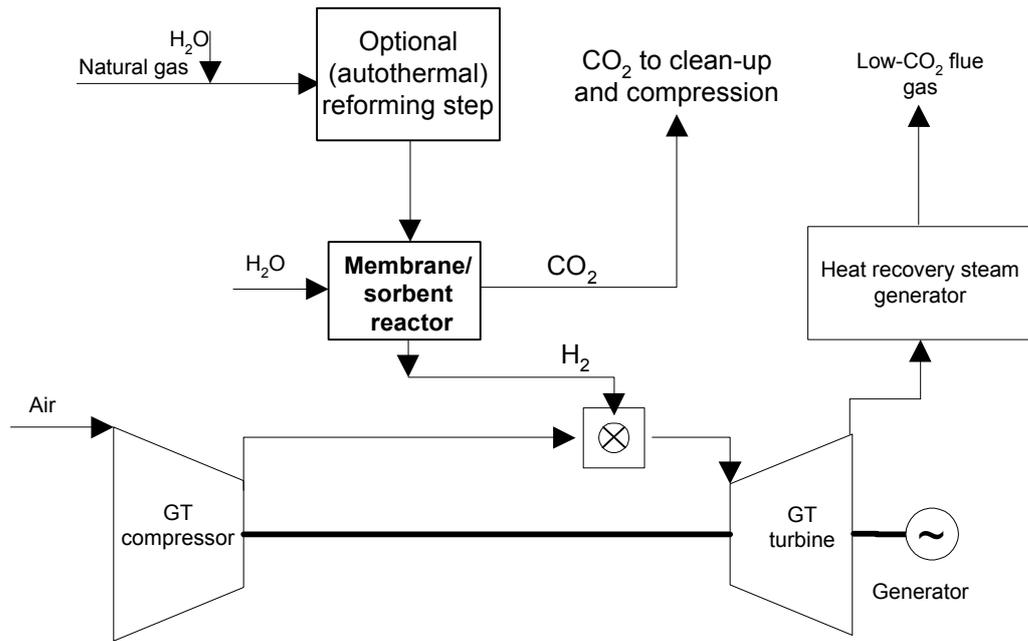


Figure 1.1: Schematic of power production from natural gas pre-combustion decarbonisation with sorbent reactors or membrane reactors.

The steam reforming (1) and the water-gas shift (2) reaction are key reactions taking place.



By removing either CO_2 or hydrogen from the reaction mixture, the reaction is shifted to the product side (separation enhanced reactions) enabling conversions in excess of thermodynamic equilibrium limitations. Effectively, the absence of a thermodynamic constraint allows a free choice of operating temperature for the separation enhanced reactions. Compared to conventional operation, the reaction temperature is lower for reforming and higher for shift. Moreover, the purity of the product is improved. This has the prospect of improving system efficiency and could also lead to investment reductions.

Summarizing the above the following options of novel pre-combustion decarbonisation reactors are considered:

- water-gas shift reactor with a H_2 membrane
- reformer with a H_2 membrane
- water-gas shift reactor with a CO_2 sorbent
- reformer with a CO_2 sorbent

1.3 Modeling tools overview

A schematic of the use of modeling tools in the CATO project is provided in Figure 1.2. The central tool is Aspen Plus. This is a flow sheeting tool in which the whole power plant is modelled thermodynamically. It provides the system efficiency, and properties of all streams in the process. It uses input from literature, experiments, detailed models and a separate gas turbine simulation program (GT-PRO). Separate from this, or integrated in Aspen Plus (for membrane reactors only) there is a sorbent or membrane reactor model used for evaluation of the performance and design of these units.

The results from Aspen Plus are used in an economic model. This estimates the main dimensions of all equipment and associated investments. It also calculates the costs of electricity and CO₂ avoided. The Aspen Icarus process evaluator is a stand-alone programme that can be used for provide input for the economic model.

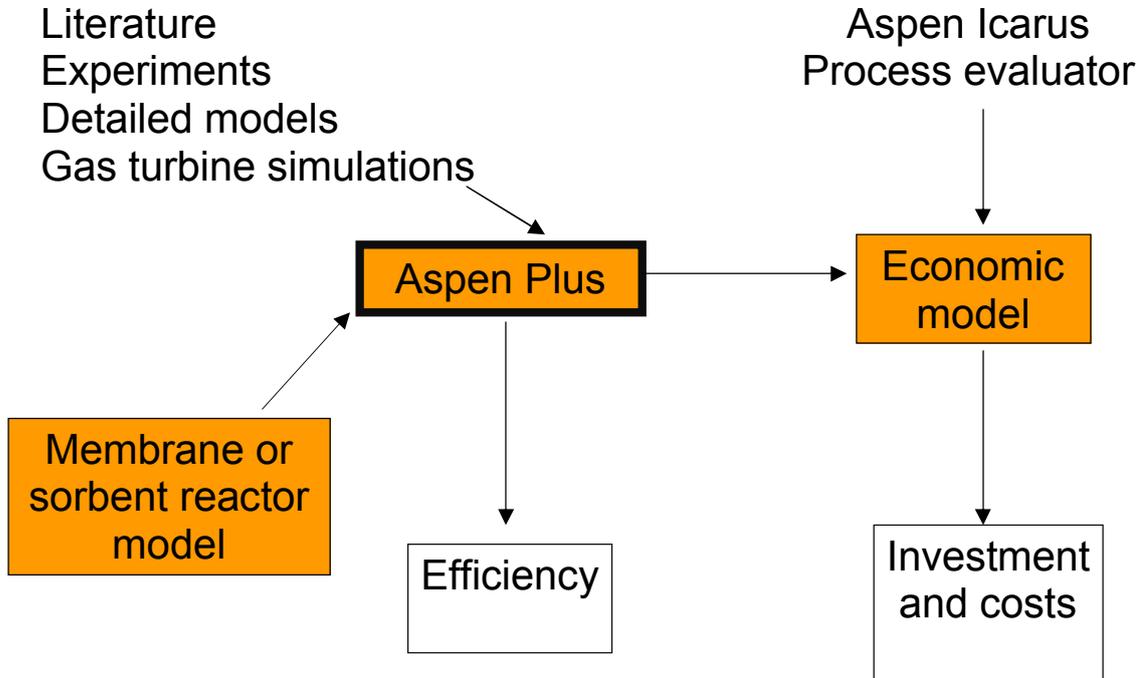


Figure 1.2: Overview of modeling tools for power plants used in the CATO project.

In this report the modeling of power plants with CO₂ capture will be evaluated. It will focus on the main tools: Aspen Plus, the membrane reactor and sorbent reactor modeling, and the economic model.

2. Modeling of membrane reactors

2.1 Membrane reactor working principle

The membrane reactor working principles for both a membrane reformer as well as a water-gas shift reactor are depicted in respectively Figure 2.1 and Figure 2.2.

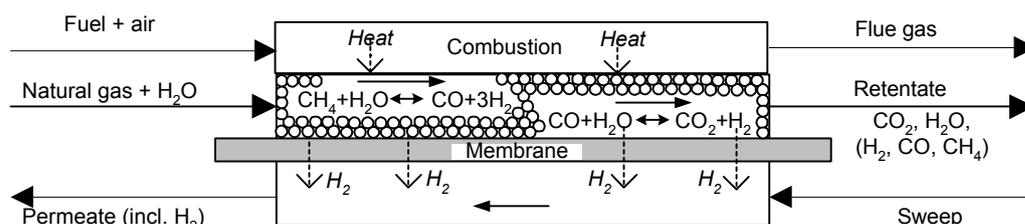


Figure 2.1: Membrane reformer working principle

The membrane reformer is fed with a mixture of natural gas and steam, which are partly converted in a pre-reforming step. The two reactions (1, 2) occurring at the feed side are respectively highly endothermic and mildly exothermic. The total reaction is endothermic, and the reaction is thermodynamically limited, thus a high temperature is advantageous for a high conversion. Parallel to the reaction, hydrogen is removed through a hydrogen selective membrane. The membrane is e.g. a supported Pd-alloy membrane. The selective removal of one of the products through the membrane (in this case hydrogen) allows for high conversion rates at relative low temperatures compared to conventional reforming. In a third combustion zone, fuel is combusted with air to provide heat to the endothermic overall reaction. The operating temperatures is around 500°C-600° C.

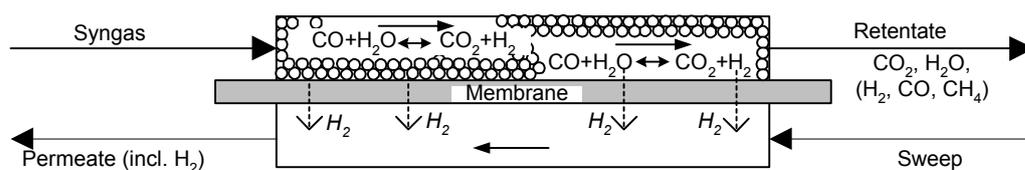


Figure 2.2: Water-gas shift membrane reactor working principle

The water-gas shift membrane reactor (see Figure 2.2) is fed with a syngas mixture from a reformer, consisting of CO, H₂, CO₂, H₂O and possibly some unconverted CH₄. The working principle is practically the same, be it that the reforming reaction does not take place. Heat supply is not necessary since the reaction is mildly exothermal; the reactor is operated adiabatically. The operating temperature is around 350-400° C, lower than that of a membrane reformer.

2.2 Description of the membrane reactor model

To design a CO₂ capture system with a membrane reactor and the reactor itself, knowledge of the impact of the main operating and design parameters on reactor performance is of great importance. To assess the impact of these parameters an in-house 1-dimensional membrane reactor model has been developed (Pex, 2005), which can be used in flow sheeting software (such as Aspen Plus). The model predicts membrane reactor performance in terms of reactant conversion and hydrogen recovery. Both are to a large extent determined by the hydrogen partial pressure profiles along the membrane reactor length on both sides of the membrane. First, the model will be described briefly, and then a summary of the results will be presented.

The membrane reactor model used is implemented in FORTRAN and operated as an Aspen Plus User Model. It takes its input directly from Aspen Plus and returns output directly to Aspen Plus.

The input/output structure is depicted in Figure 2.3. Input parameters from the flow sheeting package are the feed and sweep flow specifications, membrane surface area (A_{mem}) and catalyst volume (V_{cat}), and the heat transfer coefficient (U). In a configuration file the reaction kinetics, permeance parameters and choices for isothermal or adiabatic and co-current or counter-current operation are specified. The output of the model is permeate and retentate properties, partial pressures of all components as function of the membrane length coordinate and the heat duty in case of isothermal operation.

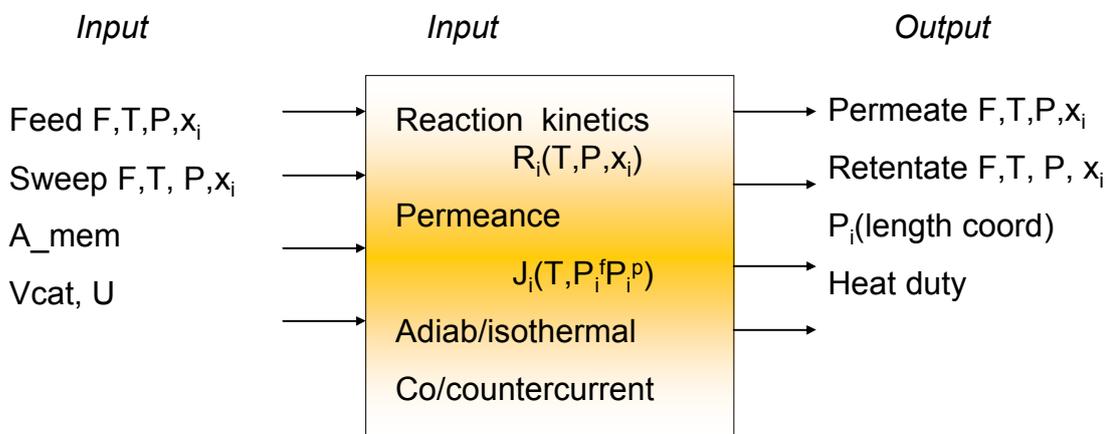


Figure 2.3: Membrane reactor model input/output structure

The following assumptions have been made:

- The model is 1-dimensional, i.e. there are no radial gradients of the concentration, velocity, pressure and temperature.
- The reactor is at steady state.
- Ideal plug flow on both sides of the membrane (no axial dispersion is present).
- There are no mass and heat transfer limitations taken into account. To some extent, these can however be included by manual adaptation of the overall permeance and/or the reaction kinetics.
- Heat can be supplied to catalyst the bed via the reactor wall, alternatively adiabatic operation is possible.
- All gaseous substances are considered as ideal gases.

The model equations are derived from microbalances of a segment along the membrane length.

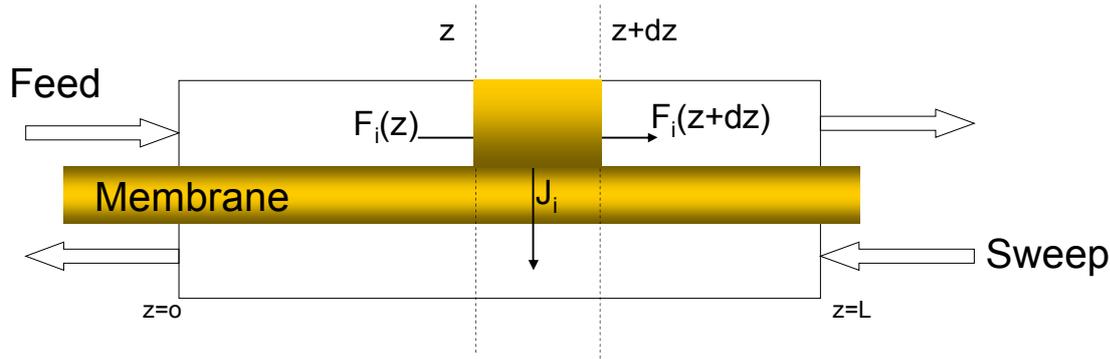


Figure 2.4: Schematic of membrane reactor model

The molar balance is specified in terms of molar flow in, out and the trans-membrane flux, production by chemical reaction:

$$F_i(z+dz) = F_i(z) - \left[\frac{A_{mem}}{L} \right] dz \cdot J_i(z, T) + \left[\frac{W}{L} \right] dz \cdot \sum_{reactions} R_i(z, T) \quad (3)$$

With F_i the molar flow of component I, z the reactor length coordinate, A_{mem} the membrane surface area, L the length, J_i the flux of component permeating through the membrane, W the catalyst mass, and rate of formation of component i .

The enthalpy balance equation can be derived in analogy with the above.

$$F_i(z+dz) \cdot h_i(z+dz) = F_i(z) \cdot h_i(z) - \left[\frac{A_{mem}}{L} \right] dz \cdot J_i(z, T) \cdot h_i(z) - \left[\frac{A_{mem}}{L} \right] U [T_f(z) - T_p(z)] \cdot Q \quad (4)$$

Where h_i is the specific enthalpy of component i , U the heat transfer coefficient and T_f and T_p the feed and permeate side temperatures, and Q the heat flux from the combustion zone. In the case of adiabatic operation Q is set zero, in the case of isothermal operation the value of Q is calculated from the heat balance. Q at the permeate side is always zero.

The trans-membrane flux is J_i described by:

$$J_i(z, T) = Q_0 e^{\left[\frac{-E_{act}}{RT} \right]} \left[P_{i,feed}^n(z) - P_{i,perm}^n(z) \right] \quad (5)$$

With Q_0 a pre-exponential factor, E_{act} the activation energy for permeance, R the gas constant, T the absolute temperature and P_i the partial pressure of component i . n is a power related to the dominating permeation mechanism.

The resulting set of equations has been rewritten as a set of partial differential equations. In the model these are solved by a library boundary value problem ordinary partial differential equation solver with a variable step algorithm. The model then returns the outcome to Aspen Plus and an Excel output file.

Figure 2.5 shows a typical result for the membrane modeling. The driving force for permeation of hydrogen is the difference of partial pressure of hydrogen between the feed and permeate side. Therefore it is interesting to plot the profiles of the partial pressure of hydrogen as the function of membrane length coordinate (=dimensionless reactor length). Figure 2.5 shows the

hydrogen partial pressure profiles along the membrane length coordinate for a typical case. At membrane length coordinate =0, the feed inlet and permeate outlet is located, at membrane length coordinate =1, the retentate outlet and sweep inlet are located. So feed flows from left to right, permeate side flow is from right to left. The difference between the feed side and permeate side partial pressure is a measure for the driving force for permeation. It can be seen that the partial pressure profiles of hydrogen on the feed side and permeate side are quite parallel for the major part of the length coordinate. This implies that the membrane flux is constant for most of the membrane length. Deviations towards higher partial pressure differences can be seen at the left and right side. The hydrogen recovery in the base case is 96.5%.

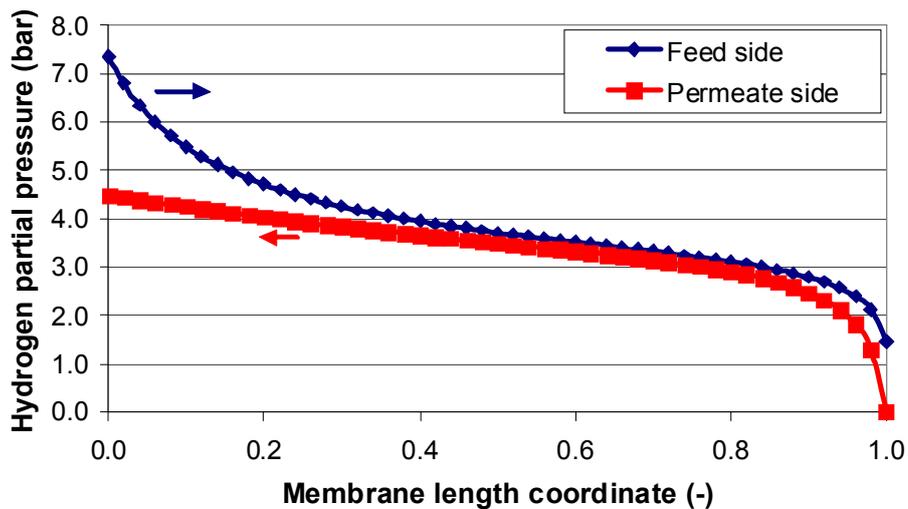


Figure 2.5: Typical example of model output for membrane reforming. Hydrogen partial pressure profiles as function of membrane length coordinate. Counter-current configuration (feed from left to right; permeate flow from right to left). Pre-reformed natural gas steam/carbon ratio=3. Pressures: 40 bar feed side, 5 bar permeate side.

3. Modeling of sorption enhanced reactors

3.1 Sorption enhanced reactors

The sorption-enhanced reaction process (SERP) offers an attractive possibility for pre-combustion CO₂ capture. Hydrogen production and CO₂ capture are combined in one step, resulting in lower capital costs.

Sorption-enhanced reaction is a batch process necessitating regeneration of the sorbent when it is saturated with CO₂. The preferred regeneration or purge gas is steam if the captured CO₂ is to be sequestered. Compared with other purge gases (air, nitrogen or methane), steam can be easily separated from the purge stream through condensation.

A simplified scheme of a sorption-enhanced reaction system for hydrogen production is shown in Figure 3.1. Two or more reactors are operated in alternating mode. Both reactors are filled with a mixture catalyst and CO₂ sorbent. In the upper reactor, natural gas and steam are converted into CO₂ and hydrogen. Hydrogen is used for power production in a combined cycle. The CO₂ is adsorbed using a solid sorbent. At the same time steam is fed to the lower reactor as purge gas for CO₂. To improve the desorption of CO₂, the temperature may be increased or the pressure may be decreased with respect to the temperature and pressure during adsorption. After the sorbent of the first reactor has become saturated with CO₂, the gas flows to both reactors are interchanged and CO₂ is desorbed from the bed of the upper reactor, whereas steam reforming is performed in the lower reactor. In the case of sorption enhanced reforming external heat supply is required, just as in a conventional steam reformer. Since the adsorption reaction is exothermic, less net heat is required. For example, for a sorbent like CaO, the adsorption heat matches the endothermic heat for the steam methane reforming reaction, and external heat supply is not required. It is also possible to include an upstream autothermal reformer to convert all the methane to CO, CO₂ and H₂ and to do only sorption enhanced water-gas shift to convert the remaining CO to H₂ with steam. For sorption enhanced water gas shift, high temperatures are not required, so this is done at much lower temperatures. For this different sorbents are used, e.g. hydrotalcites.

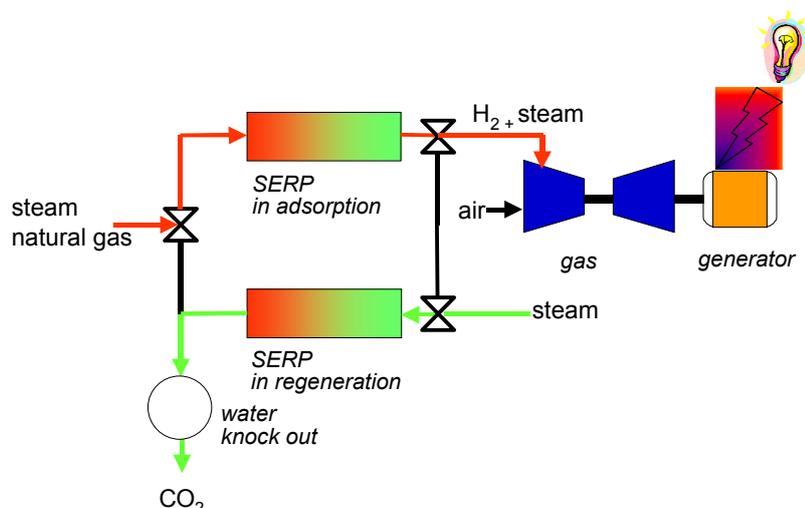


Figure 3.1: Schematic representation of natural gas combined cycle with pre combustion CO₂ capture on basis of sorption enhanced reformer reactors

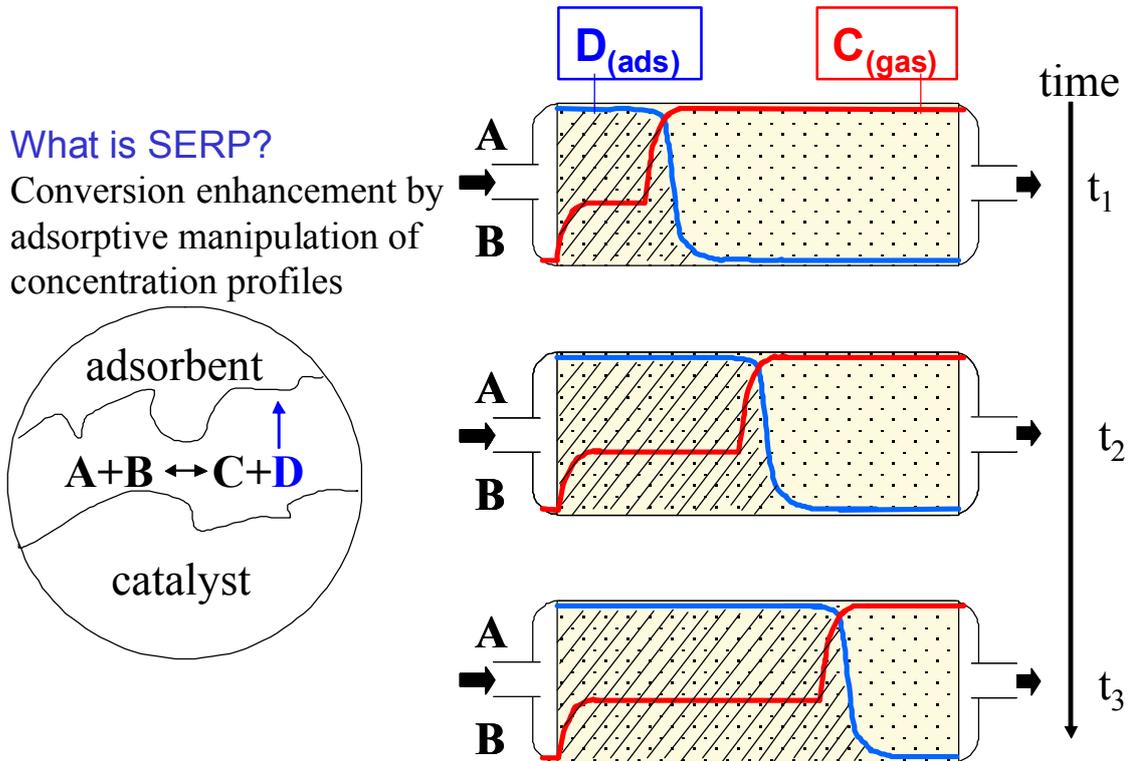
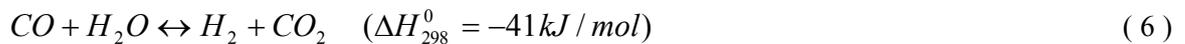


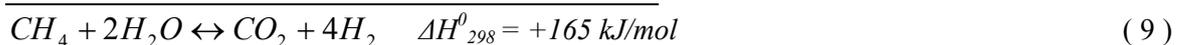
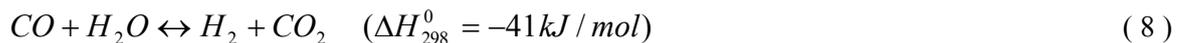
Figure 3.2: Working principle of a sorption enhanced reactor.

The working principle of sorption enhanced reaction is further illustrated in Figure 3.2. A chemical equilibrium reaction $A + B \rightleftharpoons C + D$ is performed in the presence of a sorbent, which adsorbs component D preferentially. Thus the reaction is enhanced in that part of the reactor where the adsorbent is not saturated. This part, the mass transfer zone, moves towards the end of the bed at increasing time. This is shown in the three reactor pictures where $t_1 < t_2 < t_3$.

The reaction can be either the water-gas shift (WGS) reaction only



or the steam reforming reaction followed by the water-gas shift reaction



A suitable sorbent is mixed with the catalyst. The CO_2 produced is selectively removed by the sorbent. Thus, the reaction equilibria shift to the product side, enabling the SMR and/or the WGS reactions together with the CO_2 capture processes to be combined in one single step while obtaining high conversions of the reactants. Suitable sorbent may include e.g. hydrotalcites (HTC) for water-gas shift and CaO for steam reforming.

Any system using sorption enhanced reaction should include a regeneration step to remove the adsorbed CO₂ since the sorbent is saturated after some time with CO₂. Removal of CO₂ can be achieved by purging with an inert gas, optionally in combination with a reduction of the total pressure (pressure swing) and/or an increase in temperature (temperature swing). Thus, in pressure swing mode, we have a batch process in which the reactor is periodically subject to a series of steps at different conditions for the desired processes. By using multiple reactors in parallel, a continuous product stream can be achieved, implying that the system can be integrated in a power plant with pre-combustion CO₂ capture. While one reactor is in the reaction/absorption mode, another is in desorption mode. Additional reactors are required for pressure equalizations, repressurization, rinse, blow down and purge. Thus, by using e.g. 6 reactors, it is possible to generate a continuous stream of H₂ diluted with steam for power production, and a continuous CO₂/steam stream available for storage after H₂O removal. Multiple schemes for operation of absorption/desorption cycles are possible with varying amount of reactors, these schemes can be evaluated with the model.

To predict the performance of large-scale reactors, a reactor model is needed next to the results of dedicated small-scale experiments. A model for a fixed-bed SERP reactor has been developed which includes the SMR and WGS reactions, together with a description of the CO₂ sorption process (Reijers, 2009a; Reijers, 2009b).

Reactor Model

The reactor model is a dynamic 1-dimensional reactor model. The input-output structure of the model is illustrated in Figure 3.3. The most important input data are the inlet gas properties (gas composition x_i , superficial velocity u , pressure p and temperature T) and the wall temperature. In the model are the bed properties (length and diameter, porosity, adsorbent and catalyst densities). Also, the initial conditions for the column must be specified, and in some cases some boundary conditions. In the model the reaction kinetics, adsorption isotherm and adsorption kinetics are specified. The model solves 10 variables (mole fractions of the 6 components CH₄, H₂O, H₂, CO, CO₂ and N₂, the adsorbent loading q , the superficial velocity u , the pressure p and temperature T) as a function of bed position z and time t . Thus it is possible to determine suitable operating conditions for achieving the desired H₂ and CO₂ product specs.

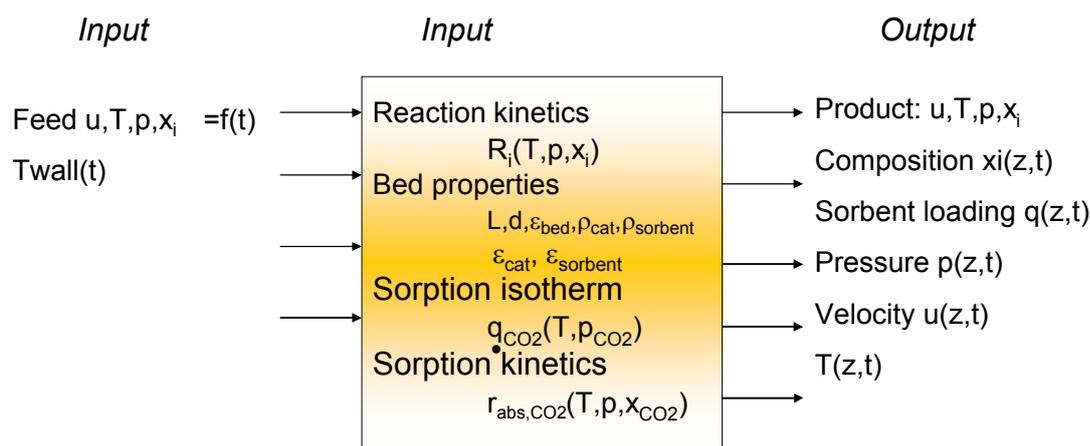


Figure 3.3: reactor model input/output structure

The following assumptions have been made:

- The model is 1-dimensional, i.e. there are no radial gradients of the concentration, adsorbent loading, velocity, pressure and temperature.
- The model is pseudo-homogeneous, i.e. the mass and heat transfer between gas and solid is so fast, that concentration and temperature differences between the two phases are negligible.

- The reactor is a tubular, fixed bed.
- Heat can be supplied to the bed via the reactor wall.
- The reactor flow is an axially dispersed plug flow.
- All gaseous substances are considered as ideal gases.
- For calculation of mass transfer coefficients and pressure drop the packing is assumed to consist of monodisperse particles. If both adsorbent and catalyst particles are present, they form a homogeneous mixture.
- The only reactions that may occur inside the reactor depending on the feed composition are the SMR and WGS reactions.
- Carbon dioxide is the only adsorbed species.
- The steady-state approximation has been used for the momentum balance equation.
- The linear driving force (LDF) approximation has been used to describe the sorption kinetics (see below).
- An effectiveness factor has been used for diffusion limitation in the catalyst.

The following equations are solved simultaneously. The mass balance reads for the six components $i = \text{CH}_4, \text{H}_2\text{O}, \text{H}_2, \text{CO}, \text{CO}_2$ and N_2 :

$$\varepsilon_t \frac{\partial c_i}{\partial t} + \frac{\partial(uc_i)}{\partial z} = \varepsilon_b \frac{\partial}{\partial z} \left(D_{\text{ax}} \frac{\partial c_i}{\partial z} \right) - \rho_{b,\text{ads}} \frac{\partial q_i}{\partial t} + \rho_{b,\text{cat}} r_i \quad (10)$$

where the sorbent loading with component i , q_i , is non-zero only for CO_2 . Here c_i is the gas phase concentration of component i , t the time, z the length coordinate, u the superficial gas velocity, ε the bed porosity, D_{ax} the axial diffusion coefficient, $\rho_{b,\text{cat}}$ and $\rho_{b,\text{ads}}$ are the bulk densities of the catalyst and adsorbent, respectively the adsorbent density, q_i the sorbent loading with component i and r_i the reaction rate, i.e. the rate of formation of component i .

The heat balance reads:

$$\begin{aligned} \frac{\partial}{\partial t} (\varepsilon_t c C_{v,\text{gas}} T + \rho_{b,\text{cat}} C_{p,\text{cat}} T + \rho_{b,\text{ads}} C_{p,\text{gas}} T) &= \frac{\partial}{\partial z} \left(k_z \frac{\partial T}{\partial z} \right) - \frac{\partial}{\partial z} (c C_{p,\text{gas}} T u) \\ &\quad - \rho_{b,\text{ads}} \Delta H_{\text{ads},\text{CO}_2} \frac{\partial q_{\text{CO}_2}}{\partial t} + \rho_{b,\text{cat}} \sum_i H_i r_i \quad (11) \\ &\quad + \frac{4U}{d_t} (T_w - T) + \varepsilon_t \frac{\partial p}{\partial t} \end{aligned}$$

with C_v , C_p the heat capacities, T the temperature, k_z the axial thermal conductivity, ΔH_{ads} and ΔH_r the heat of adsorption and reaction, respectively, U the heat transfer coefficient d_t the tube diameter and p the pressure.

The momentum balance reads

$$\frac{\partial p}{\partial z} = -K_D u - K_V u |u| \quad (12)$$

with K_D and K_V constants as defined in the Ergun equation.

To solve for the 10 variables, two additional equations are needed, obtained by summing Equation 10 over all six components:

$$\varepsilon_t \frac{\partial c}{\partial t} + \frac{\partial(uc)}{\partial z} = -\rho_{b,ads} \frac{\partial q_{CO_2}}{\partial t} + \rho_{b,cat} \sum_i r_i, \quad (6)$$

where $c = \sum_i c_i$ has been used, and the relation for the linear driving force (LDF)

$$\frac{\partial q_{CO_2}}{\partial t} = k_{LDF} (q_{CO_2}^* - q_{CO_2}), \quad (7)$$

where $q_{CO_2}^*$ is the equilibrium CO₂ loading of the adsorbent, q_{CO_2} is the actual CO₂ loading averaged over the particle volume, and k_{LDF} is a lumped parameter for the sorption rate of CO₂ by the particle taking into account all mass transfer.

The partial differential equations are discretized in the axial direction using the second order upwind scheme for the convective terms and finite differences for the second-order terms. The remaining set of time-dependent ordinary differential equations is solved by a finite difference method using a Matlab software package.

The adsorption process is described using adsorption isotherms, e.g. a Freundlich isotherm given by:

$$q_{CO_2}^* = k \left(\frac{p_{CO_2}}{101325} \right)^{1/n} \quad (13)$$

where $q_{CO_2}^*$ denotes the equilibrium loading and p_{CO_2} , expressed in Pa, the partial CO₂ pressure. The parameters k and n (with $n > 1$) are fit parameters determined by fitting the model isotherm to the experimentally obtained data.

In the regeneration stage, the reaction kinetics are disregarded and the desorption of CO₂ from the sorbent can be simulated.

A typical example of a model output of simulation of sorption enhanced reaction simulation is provided in Figure 3.4. It can be seen that the CO₂ loading is initially very low, and then increases with time, starting at the entrance of the reactor (left hand side). The CO₂ loading at the reactor outlet (right hand side) has a tail-shaped curve, with a gradual increase of the height of the tail with time, until the sorbent is fully loaded with sorbent. Since this is a very short lab scale reactor, breakthrough of CO₂ in the product gas is quite early, compared to the time necessary for full loading of the sorbent. For a much longer full scale reactor it will take relatively much more time before CO₂ breakthrough is significant.

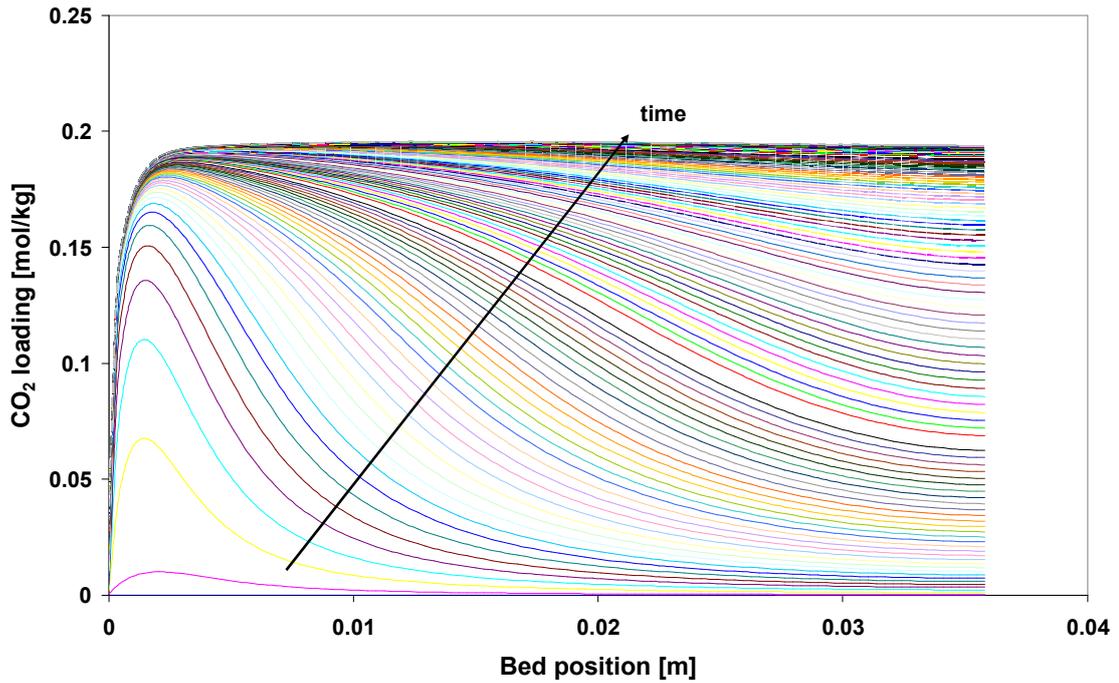


Figure 3.4: Example output of the sorption enhanced reaction model: CO_2 loading as a function of bed position for various times. The arrow indicates increasing time. Sorption enhanced reforming at 400°C , 1 atm.

Feed 5.8% CH_4 , 17.2% H_2O , balance N_2 wet flow 25 ml-STP/min, Reactor diameter: 1.6 cm, Catalyst mass: 3.0 g, Adsorbent mass: 2.2 g (commercial MG70 promoted with 22 wt% K_2CO_3). The Freundlich isotherm has been used with $k = 0.7 \text{ mol/kg}$ and $1/n = 0.3$.

4. Flowsheet modeling of power plants with CO₂ capture

This chapter describes the tools and methodology of system assessment studies that were performed for complete power plants with CO₂ capture. These studies were conducted by designing flow sheet models and evaluating their results. Before the system assessment studies within the CATO project will be discussed, we will first elaborate on the general benefits of system assessment studies (see Figure 4.1 for an overview).

4.1 Reasons for system assessment studies

As is observed in the previous chapters, there are several novel ideas to produce power with pre-combustion CO₂ capture. In this particular case we are not dealing with a single idea, but with several. To gain in depth knowledge of all options would require the investment of a significant amount of time and effort. Before starting such elaborate research, it is also possible to scan the potential of different options. By comparing the different ideas we can assess which processes are the most promising. This could guide us in the selection of processes which will be researched more in depth. Therefore, system assessment studies are a means of guiding research and development. The primary aspects here are of course the calculated system efficiency, but also the process conditions required and the magnitude of flows and size of equipment.

There is a second way in which system assessment studies guide research. When modeling complete systems it becomes apparent which parameters play an important role in the process in terms of efficiency, equipment sizing, and operating conditions. Based on this information it can become clear which are the bottlenecks expected with a new technology and where potential improvements can be achieved. In that way the system assessment studies can guide subsequent research.

Finally, system assessment studies will give the required input for economic evaluation. The economics of chemical processes depend on many different aspects. Clearly, the type of equipment and cost of catalysts and raw materials will influence the process economics. But other aspects are important as well, like the parasitic power requirement, use of utilities and the required manpower for operating a plant. Knowledge of the system will provide valuable input for subsequent economic evaluations and is thus a clear reason for performing system assessment studies.

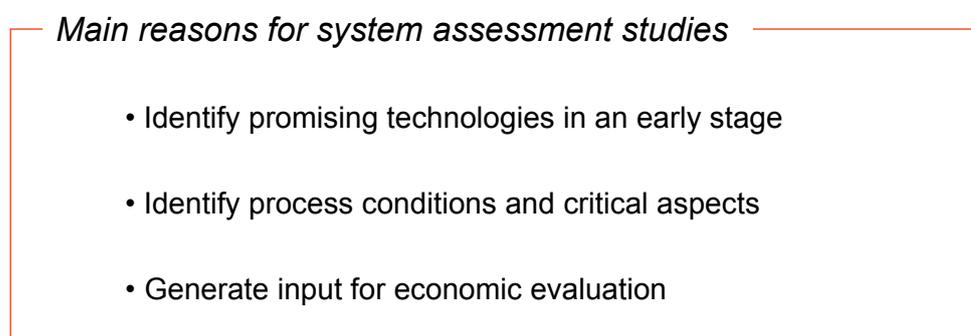


Figure 4.1: *Overview of the main reasons for utilizing system assessment studies*

4.2 Using Aspen Plus for system analysis studies

It was chosen to utilize Aspen Plus (Aspentech, 2009) to perform the system analysis studies. Aspen Plus is a process modeling tool for conceptual design, optimization, and performance monitoring of chemical processes. Aspen Plus predicts process behavior using engineering relationships such as mass and energy balances, phase and chemical equilibrium, and reaction kinetics. With reliable thermodynamic data, realistic operating conditions, and the rigorous equipment models, one is able to simulate actual plant behavior.

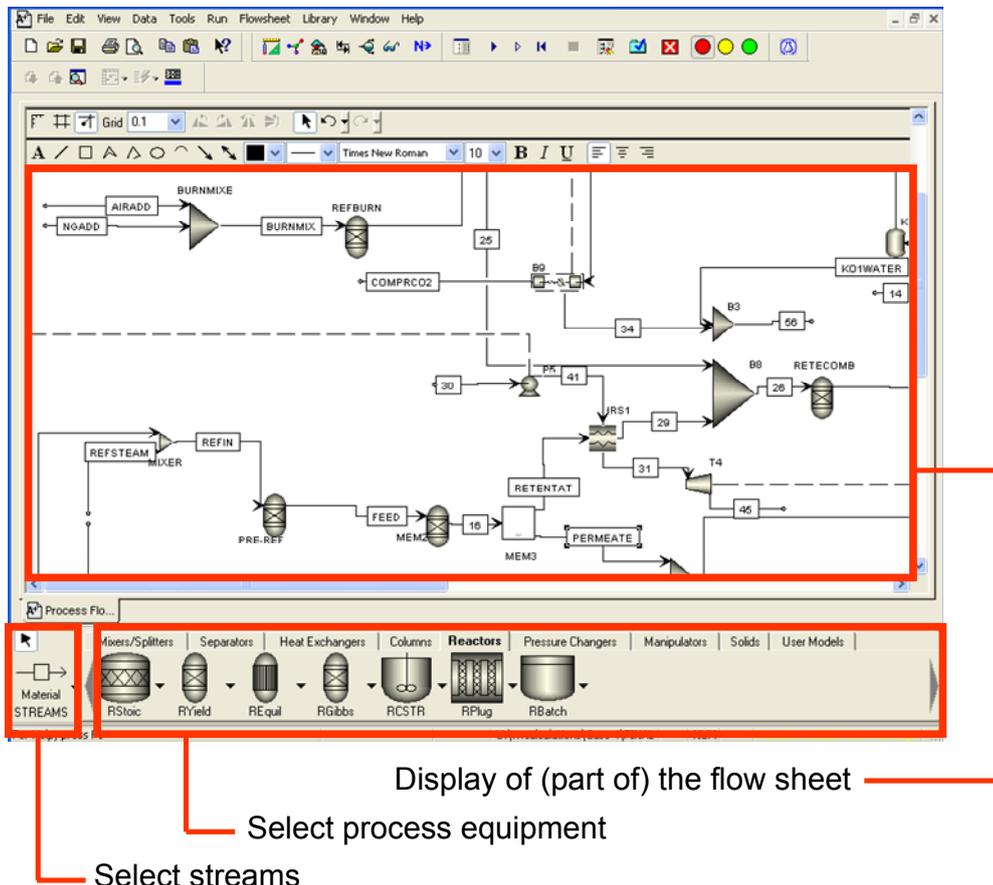


Figure 4.2: Example of an Aspen Plus file including a brief explanation of main elements

In Figure 4.2 an example of an Aspen Plus model is given. It can be observed that a flow sheet can be modeled relatively easy, as there is a menu to select streams and process equipment. Aspen Plus contains a comprehensive library of unit operation models, including solid, liquid and gas processing equipment. Furthermore, Aspen Plus contains a large database of pure component and phase equilibrium data for conventional chemicals, electrolytes, solids and polymers.

4.2.1 Modeling of power plants with CO₂ capture

The processes to be evaluated with Aspen Plus within the CATO project were partly composed of standard pieces of equipment that could be readily modeled by means of the equipment library (e.g. pumps, compressors, heat exchangers). However, the processes also contained specialized pieces of equipment (e.g. membrane water-gas-shift reactors, sorption enhanced reformer reactors). Obviously, in the standard process equipment library of Aspen Plus these types of equipment are not featured. This problem was tackled in two ways:

- In some cases it was chosen to incorporate the detailed models that were made of the specialized equipment. For instance, the FORTRAN model of the membrane reactors was used in

the Aspen Plus simulations. The open environment of Aspen Plus allows custom or third-party models inside an Aspen Plus simulation.

- In other cases it was chosen to model specialized equipment in Aspen Plus by using a combination of the available process equipment in the Aspen Plus library. For instance, this was the case for the Sorption enhanced shift reactor. This piece of equipment was modeled by a combination of a splitter and a reactor. The input for this model was obtained by a combination of literature data, experiments and detailed reactor modeling. Another example is the modeling of the gas turbine. Here input data was obtained from a full gas turbine model in the simulation program of GT-PRO. This data was utilized in a simple Aspen Plus model consisting of a compressor, a burner and a turbine with constant input parameters.

4.2.2 Two-step approach to system studies

In the system studies a two-step approach was used. First the systems were assessed by more general, simple models. The second phase is an extension of the models, going more into detail and adding complexity (see Figure 4.3).

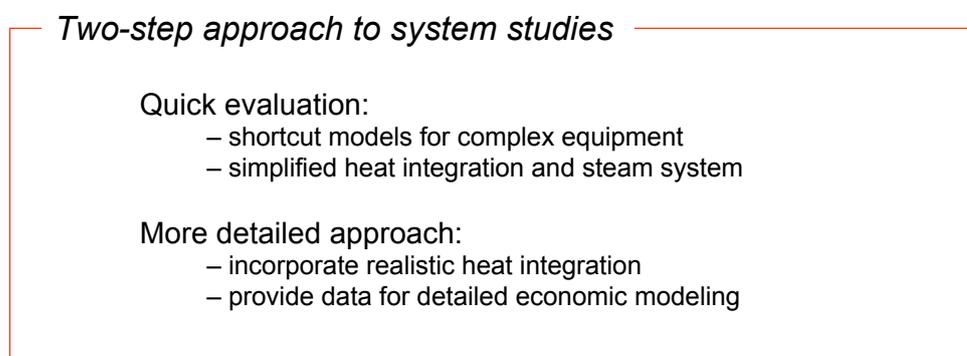


Figure 4.3: Overview of the two-step approach in system studies

A characteristic of the models in the first phase is the fact that shortcut models are used for complex equipment. (This aspect was addressed in the previous paragraph.) By giving a simplified representation of complex equipment in the system studies, it is easier and faster to model the systems, making it possible to do a quick evaluation.

Another characteristic of these first phase models is simplified heat integration. Instead of evaluating different possible methods of heat integration for each system (including multiple heat exchangers), it was chosen to simplify heat integration in Aspen Plus. Use was made of the heat exchanger 'MHeatX' in the equipment library of Aspen Plus, which allows heat transfer between multiple hot and cold streams (see Figure 4.4). An advantage of this heat exchanger is the fact that it can be modeled without specifying exactly how the hot and the cold streams are matched. In this way the maximum heat transfer possible in the system can be assessed (pinch method) by modeling only one heat exchanger for the entire process.

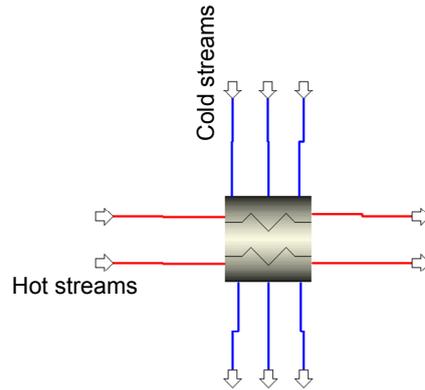


Figure 4.4: Example of simplified heat integration in Aspen Plus.

Finally, a simplified steam system was used. In general, power plants apply steam at different pressures: high, intermediate and low. In the first phase of the system studies it was chosen to model the system with steam at only one pressure. This allows for much more rapid evaluation of systems. In addition, there is no offset created by insufficient optimization of a complex steam system. Of course, one concept could benefit a bit more for the simplification made than another concept.

In phase two of the system studies, the models were more detailed and complex. For heat integration, realistic setups were modeled consisting of several heat exchangers, instead of the MHeatX heat exchanger model. Also, ‘forbidden’ matches were taken into account, which are combinations of hot and cold streams that are not possible for e.g. safety considerations (such as heating a natural gas stream with a hot oxygen containing flue gas stream). Also, the impact of metal dusting is accounted for. This implies that reducing streams can only be cooled by generating saturated steam (not superheated steam) to limit the wall temperature of the heaters involved. These adaptations increase the knowledge of the system and yield data for more detailed economic models. For the equipment more detailed models, or results from experiments are used, though occasionally also shortcut models are applied.

5. Economic evaluation of CCS systems

Because of the large number of process cases to be examined, it was impossible to make very accurate cost calculations based on a basic design of all the processes and on price quotations of main equipment. Therefore a quick, but also less accurate, costing method has been used with an estimated inaccuracy of approximately 30%.

All estimated costs have been based on information of 2006 and have been expressed in euros. When earlier data had to be used, an average inflation rate of 2% per year has been applied.

5.1 General Model Structure

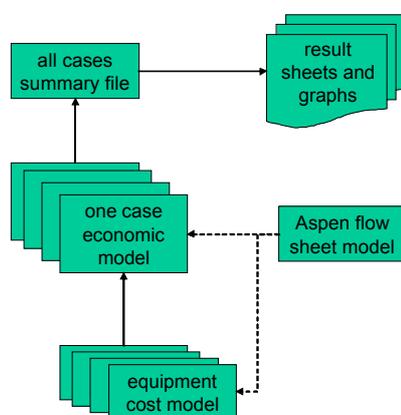


Figure 5.1: *Cost Model Structure*

The main cost model structure is shown in Figure 5.1 and can be explained in the following way.

The model can evaluate multiple cases (e.g. different process configurations), that can be compared with each other. For each case a “one case economic model” has been created as an MS Excel workbook with a standard content of worksheets:

1. General starting points
2. Case specific process data
3. Investments
4. Cash flow time series
5. Main results

For the starting points we have followed the IEA GHG starting points (IEA GHG, 2003) as much as possible. The complete list of general starting points is shown in the appendix. These include construction period specifications, the expenditure scheme, plant life time assumptions, load factors, discount rates, contingencies and assumptions for tax, maintenance costs etc.

For the investment estimation, a bottom-up cost information flow has been applied. So, first equipment costs have been estimated with information from the Aspen Plus flow sheet simulations as described in chapter 4. Therefore standardized “equipment cost models” have been used and integrated into the “one case economic model”. Then these equipment costs have been dynamically linked to the sheet: Investments and have been totalized as will be explained in the next section.

Cash flows have been calculated based on: i) the general starting points, ii) the case specific process data, like power output, net electrical efficiency and CO₂ capture efficiency, and iii) the total investment costs. The main results of the cash flow calculations have been summarized on a separate worksheet in the “one case economic model”.

Finally the main results of all CCS cases have been taken together in the “all cases summary file”, a separate MS Excel workbook, via dynamic links to make a quick and actual comparison of all cases possible.

5.2 Estimating investment costs

Plants are assumed to be build in North-East of the Netherlands, within 1 km off the coast. A greenfield site has been assumed. Utilities and infrastructure are outside the battery limits.

All the processes examined are power plants with or without extra equipment for the pre-combustion capturing of CO₂. The whole plant can be divided into three different types of components:

- standard process equipment needed for CCS, like heat exchangers, pumps, compressors, vessels etc.;
- special devices or materials needed for CCS, like: membranes, a catalyst or an adsorbent bed.
- standard power plant components, like: a gas turbine, a steam turbine cycle or a heat recovery steam generator etc.;

For these types of equipment different ways of cost estimation have been followed, as discussed in the next paragraphs.

5.2.1 Standard process equipment

For the standard process equipment we have used as much as possible the cost information of DACE, the Dutch Association of Cost Engineers (Dace, Webci& Wubo, 2006; Holt, 1998) . This cost information has been translated into equipment cost models, written in MS Excel, for each relevant type of equipment. The required process parameters, like the power demand of a compressor or the duty and temperatures of a heat exchanger, have been calculated in the Aspen Plus flow sheet simulations and have been copied manually into these equipment cost models, leading to a cost estimation for that specific piece of equipment.

5.2.2 Special Devices and Materials

The cost information of the special devices and materials is ECN’s in-house information coming from research specialists. When possible, a consistency check with public information has been carried out.

5.2.3 Standard Power Plant Components

Standard power plant components have been regarded as package units for which specific investment costs have been used, as mentioned in literature. The specific investment costs, found in literature, have been related to the real capacity or duty as calculated in the Aspen Plus flow sheet simulations, leading to the total costs for all power plant components. Scaling has been done according to the Williams rule, using scaling exponents from (Peters, Timmerhaus& West, 2003). For currency conversion assumptions see Appendix B. Past year data have been converted to the assumed investment basis year (year 2006) using a 2% depreciation rate.

5.2.4 Total investment costs

To get the total investment cost one has to add several surcharges to the equipment costs. For standard process equipment several surcharges have been taken into account. For this we have used the so called Lang factors, as described in (Peters, Timmerhaus& West, 2003). These surcharges on the bare equipment costs are:

Installation surcharge	47%
Instrumentation surcharge	36%
Piping surcharge	68%
Electrical equipment surcharge	11%
Buildings surcharge	18%
Service facilities surcharge	15%

However, we have lowered the service facilities surcharge from 70%, as mentioned in (Peters, Timmerhaus& West, 2003), to 15%, because the necessary power plant buildings have already been taken as part of the standard power plant components, see paragraph 1.1.3.

The bare equipment costs together with these surcharges are called the direct investment costs. For the standard process equipment extra surcharges have been taken into account, the so-called indirect investment costs. These surcharges, on top of the direct investment costs, are:

Engineering and supervision surcharge	9%
Construction and supply surcharge	11%
Contractor's fee surcharge	6%
Contingency surcharge	12%

Special devices and materials can be rather expensive catalysts, membranes etc., for which it is not reasonable to increase these costs by using the direct investment surcharges. For instance, when a reactor vessel is filled with a very expensive noble metal catalyst, it would not be realistic to assume proportionally additional costs for piping, instrumentation, civil works etc. Therefore these surcharges are not taken into account for the catalyst. The reactor vessel and the normal surcharges for it are accounted for in the 'standard equipment' section. However, the indirect surcharges, like for engineering, construction and contractors fee, have been applied indeed.

For the power plant components, to be realized as package units, we have used data in which the investment costs are all inclusive. That means that not only costs for the related piping, instrumentation, electrical equipment and civil construction, buildings, but also costs for engineering, procurement, assembling, contractors fee and contingency have already been taken into account within the specific investment costs of these large components. So no surcharges have been added for these components at all.

5.3 Cash Flow Calculations

For the cash flow calculations time series have been set up on a separate worksheet in the CCS case workbook.

Based on the general starting points, the case specific process data and the total investment costs of that case all fixed and variable costs and benefits have been calculated as function of time for the total economic lifetime of the power plant, leading to a net cash flow for each year. Also the electricity costs for each year are calculated. See Appendix B for the assumptions.

Assuming an electricity selling-price, and calculating the future value of revenues and costs to present day, one can calculate the net present value of the plant. Or, in an alternative approach, one can calculate the electricity price leading to a break even (NPV=0).

By comparing these results with the performance of the same type of power plant but without CCS, one can calculate the differences in CO₂ emissions and electricity costs, leading to the specific costs per ton avoided CO₂ emission.

5.4 Criteria

The main results of the cost calculation of each case are transferred to the “all cases summary file”, providing a quick overview. These main results are:

- Net Plant Power Output
- Net Efficiency
- CO₂ capture efficiency
- Total Investment Costs
- Specific investment costs
- NPV of total cash flow (with electricity price of 50 Euro/MWh)
- Cost of Electricity without CCS
- Cost of Electricity with CCS
- Captured CO₂ per MWh
- Avoided CO₂ per MWh
- Specific Captured CO₂ Costs
- Specific Avoided CO₂ Costs

One could choose different approaches for comparison of the cases.

Striving for the biggest CO₂ emission reduction, of course the specific avoided CO₂ costs is an important criterion. However, the investor has still to accept the total investment of that plant. Looking for sustainability, the highest net efficiency is of paramount importance, while for the business the lowest cost of electricity will be decisive.

6. Conclusions and evaluation

For analysis of pre-combustion decarbonisation reactors and zero emission power plants a set of modeling tools is available. The tools are used to assess the technical and economic feasibility of reduction of the energy penalty associated with CO₂ capture. The tools give a vast variety of information varying from the thermodynamic and economic potential, boundary conditions for operation of unit operations to detailed understanding of important phenomena in equipment used in CO₂ capture processes.

The central tool is Aspen Plus. This tool gives the thermodynamic efficiency of the power generation plant. A two-step approach gives the choice between a doing a quick survey of process conditions an efficiency potential, or a more detailed study giving input for economic evaluation while including practical limitations in heat integration design. The latter gives a more reliable choice but the experience is that the modelling effort required is much larger.

The results from Aspen Plus form the input for an economic evaluation model. Using standard equipment evaluation sheets and custom methods for specialized equipment the investments of a power plant are obtained. Using a time value of money approach then the price for CO₂ avoidance is calculated.

For membrane reactors a 1-dimensional model for sizing of a membrane reactor is available. This model simulated reaction and permeations, and accounts for depletion along the reactor length. The combination of this model with Aspen Plus gives the opportunity of assessing the important trade-off between equipment size (and fixed costs) vs. efficiency (variable costs). Present in membrane systems design.

For sorbent reactors a 1-dimensional model is available that simulates the (time dependent) cyclic process in sorbent reactors. The model gives information on the required equipment size, but also on the important amount of steam required for regeneration (purge).

The combination of the thermodynamic modeling with the special equipment models proved to be valuable. It gives insight in the optimal design conditions and provides guidance for development of the membrane reactors and sorbent reactors, as well as info on (non-)feasible process options and on the thermodynamic economic and economic potential.

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Appendix A Starting points for system evaluations

A.1 System size and application

Table 1 lists the main properties of the systems that are evaluated in this study. The systems are based on a combined cycle unit consisting of a single shaft Siemens V94.3A gas turbine and a single steam turbine, mounted on the same shaft (this single shaft lay out is not very important as rotational speeds in particular and off-design behaviour in general are not taken into account). The systems will be evaluated for electricity production (with or without CO₂ capture) only. Heat production will not be valued.

Table 1: *General system starting points*

System characteristics	
Power production (without CO ₂ capture)	Approx. 380 MWe
Goal	Electricity generation
Heat production	Not valued
Location	The Netherlands

A.2 Feed and product specifications

Feed streams for all systems are natural gas, air and water. All systems run on 40 bara natural gas, having a composition based on (IEA GHG, 2000). The only difference is that H₂S is not taken into account. Feed specifications are listed in Table 2 and Table 3.

Table 2: *Natural gas specifications*

Property	Value
Composition:	vol.%
CH ₄	83.9
C ₂ H ₆	9.2
C ₃ H ₈	3.3
C ₄₊ (as C ₄ H ₁₀)	1.4
N ₂	0.4
CO ₂	1.8
Lower heating value (LHV)	46.899 MJ/kg
Pressure	40 bar
Temperature	15 °C

Table 3: *Feed air specifications*

Property	Value
Composition:	mole%
N ₂	77.29
O ₂	20.75
H ₂ O	1.01
Ar	0.92
CO ₂	0.03
Temperature	15 °C
Pressure	1.013 bar

Table 4: *Products specifications*

Product	Specifications
Useful power	Shaft power delivered by turbines
Heat	temperature as available, not valued
CO ₂ for sequestration	Pressure = 110 bar Temperature = 50° C

A.3 Process equipment specifications

Table 5, Table 6, and Table 7 present the specifications of the process equipment as they are used in the simulations and in the equipment sizing. No pressure losses are assumed to occur inside the equipment.

Table 5: *Fuel treatment and membrane reactor process equipment specifications system 1*

Type	Default
Reformer	
Aspen component	RGibbs*
Temperature	850 °C
Species taking part in reactions (rest inert)	CH ₄ , N ₂ , CO ₂ , Ar, H ₂ O, H ₂ , CO, O ₂
Steam to carbon ratio	3.0 mole/mole
Pre-shift	
Aspen component	RGibbs*
Species taking part in reactions (rest inert)	CO, H ₂ , CO ₂ , H ₂ O
Duty	0 (adiabatic)

*RGibbs: Gibbs minimization equilibrium reactor

Table 6: *Fuel treatment and membrane reactor process equipment specifications system 2*

Type	Default
Prereformer	
Aspen component	RGibbs*
Species taking part in reactions (rest inert)	CH ₄ , N ₂ , CO ₂ , Ar, H ₂ O, H ₂ , CO

*RGibbs: Gibbs minimization equilibrium reactor

Table 7: *Remaining process equipment specifications system 1 and 2*

Gas turbine compressor section	
Gas turbine inlet flow	627.21 kg/s
Isentropic efficiency η_{is}	0.865
Pressure ratio	16.9
Gas turbine combustion chamber	
Pressure loss	0.51 bar
Heat loss	2 MW
Gas turbine expander section	
(Max.) Inlet temperature	1238.5 °C
Isentropic efficiency η_{is}	0.902
Discharge pressure	1.03 bar
Steam cycle section	

Steam turbine isentropic efficiency	0.90*
Steam turbine discharge quality	0.90
Condensor outlet pressure	0.040 bar
Condensor outlet temperature	25 °C
HRSG Pinch temperature	5 °C
Hot end approach temperature HRSG	35 °C
Pump efficiency	0.8

Retentate conversion and CO₂ compression section

Retentate turbine discharge pressure	1 bar
Retentate turbine isentropic efficiency	0.85
Number of CO ₂ compression stages	5
Isentropic efficiency compressors η_{is}	0.85
Interstage cooling temperature	50 °C
Exit temperature T _p adjustment	20 °C

*Value for a single steam turbine. If split up in separate high-pressure and low-pressure steam turbines, isentropic efficiencies per turbine are slightly less (here 0.88664 used).

Appendix B Assumptions for economic valuations

General assumptions

(in accordance with IEA GHG technical and financial conventions, rev B2, July 2003)

Input variables	calc. value	unit
<i>Construction Period</i>		
plant type	gas fired	
constr period coal fired power station		3 year
constr period gas fired power station		2 year
constr period CO2 capture plant		2 year
constr period chemical plant		2 year
first year of operation		2010 year
<i>Expenditure Scheme</i>		
1st yr expend. coal fired PP	20%	%
2nd yr expend. coal fired PP	45%	%
3rd yr expend. coal fired PP	35%	%
1st yr expend. gas fired PP	40%	%
2nd yr expend. gas fired PP	60%	%
1st year expend. chemical plant	40%	%
2nd year expend. chemical plant	60%	%
<i>Plant Life</i>		
power plant life		25 year
<i>Load Factor</i>		
start-up time		3 month
1st yr load factor coal solid liquid plant	60%	%
nxt yr load factor coal solid liquid plant	85%	%
load factor gas fired plant	90%	%
<i>Capital Charges</i>		
discount rate	10%	%
<i>Contingencies, Fees, Owner Costs</i>		
general contingency on plant investm	10%	%
fees and owner costs	7%	%
<i>Taxation and Insurance Costs</i>		
local tax rate based on plant investm	1%	% per year
insurance costs based on plant investm	1%	% per year
<i>Maintenance Costs</i>		
maintenance costs solids handling	4%	% per year
maintenance costs gas handling	2%	% per year

General assumptions

(in accordance with IEA GHG technical and financial conventions, rev B2, July 2003)

Input variables	calc. value	unit
<i>Labour, Supervision and Administration Costs</i>		
number of operators gas fired plant	3	#/shift
number of operators coal fired plant	5	#/shift
number of shifts	5	# shifts/day
labour costs per fte	\$50,000	USD/year
supervision allowance	20%	
administration allowance	30%	
<i>Fuel Prices</i>		
coal price 2003	2	Euro/GJ
gas price 2003	5	Euro/GJ
coal price yr increase	1	factor
gas price yr increase	1	factor
<i>Product Prices</i>		
Electricity Price	50	Euro/MWh
By-product price	105	USD/ton
<i>Currencies</i>		
US dollar rate	1.35	Euro/USD
<i>Investment surcharges on equipm costs</i>		
Installation surcharge	47%	%
Instrumentation surcharge	36%	%
Piping surcharge	68%	%
Electrical equipment surcharge	11%	%
Buildings surcharge	18%	%
Service facilities surcharge	15%	%
<i>Investment surcharges on direct inv csts</i>		
Engineering and supervision surcharge	9%	%
Construction and supply surcharge	11%	%
Contractor's fee surcharge	6%	%
Contingency surcharge	12%	%
<i>Chemicals, Consumables and Waste Disposal</i>		
Waste disposal cost (2003)	7	USD/ton
Waste disposal cost	0.0055	Euro/kg
<i>Specific CO2 emissions</i>		
Specific CO2 emission coal	94	kg/GJ
Specific CO2 emission NG	56	kg/GJ