Deliverable nr D303
Helsinki 2012

Timo Laukkanen

Aspen Dynamics as a dynamic simulation tool for oxyfuel power plants

CLEEN LTD
ETELÄRANTA 10
P.O. BOX 10
FI-00130 HELSINKI
FINLAND
www.cleen.fi

ISBN XXX-XX-XXXX-X
ISSN XXXX-XXXX

Abstract

In this report the objective is to study the possibility to use AspenDynamics as a dynamic simulation tool to study the dynamic behavior of oxyfuel combustion processes. An important part is to study how existing AspenPlus models can be transformed into AspenDynamics models. This has been accomplished by studying simplified examples of parts or the total oxyfuel combustion process. The objective has not been to develop a fully realistic process based on a well-defined case nor has the objective been to study the dynamic behavior in detail and in different operating conditions or to develop a fully working control system for the process. These issues will be studied later during the project. According to the knowledge gained by the four models developed for testing, it can be concluded that AspenDynamics can be used to study the dynamic behavior of oxyfuel combustion processes, although in some situations this can be tedious and hard to accomplish. In the future, the main focus will be on developing an detailed AspenPlus model of a specific case study. This model will be then transformed into a detailed AspenDynamics model, which is used to study the dynamic behavior of different operational conditions of oxyfuel combustion processes.

Contents

0.1 Introduction

The problem of global climate change has brought forward the question of reducing significantly greenhouse gases, especially CO_2, emissions into the atmosphere. One option to accomplish this is CO_2 capture and storage (CCS). This way fossil fuels, especially coal, could be used as a fuel in power production and with no or limited emissions to the atmosphere. The problem is that the costs of power production would increase and research is needed to find a suitable and trustworthy storage place for the CO_2. The sequestration could be done with pumping the gas into oil wells or salt aquifers or with mineral carbonation. The capturing could be done with three major technologies: post-combustion capture systems, precombustion capture systems and oxyfuel combustion capture systems.

In this report the focus has been one oxyfuel combustion processes, although in general the simulation tools used could also be used in other CCS technologies. During oxyfuel combustion, a combination of oxygen (typically of greater than 95% purity) and recycled flue gas, i.e. not air, is used for combustion of the fuel. A gas consisting mainly of CO_2 and H_2O is generated. This flue gas has a CO_2 concentration high enough for sequestration, although typically the CO_2 is purified and liquefied in a subprocess called Gas Purification Unit (GPU). The recycled flue gas is used to control flame temperature and make up the volume of the missing N_2 to ensure there is enough gas to carry the heat through the boiler. O_2 is separated from air in a subprocess called Air Separation Unit (ASU). The GPU and ASU are the major contributors to an efficiency penalty of about 7-12 %-points compared to a power plant without CCS.

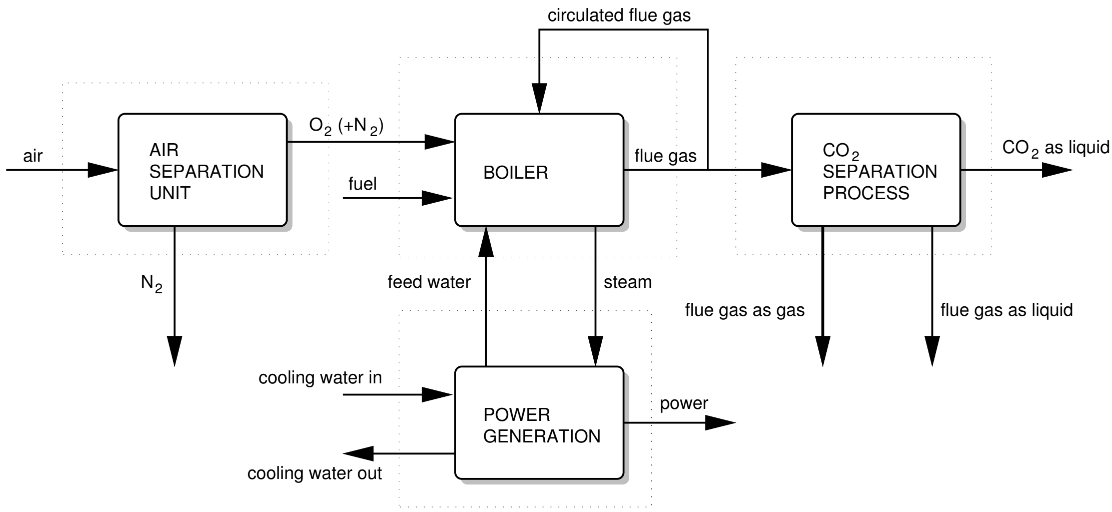

Figure 1: Oxyfuel power plant concept

Steady-state process simulations provide the opportunity to design and optimize processes so that they are in mass- and energy balance. This can be done in a cost-efficient and safe way by using computers. On the other hand dynamic process simulation provides the opportunity to study the dynamic behavior of these processes providing the opportunity to

- understand and solve operational problems
- improve operability
- increase process safety
- ensure environmental performance
- ensure product quality
- understand and improve process start-ups and shut-downs
- improve process control

AspenPlus [1] from AspenTech is a market-leading process modeling tool for conceptual design, optimization, and performance monitoring for the chemical, polymer, specialty chemical, metals and minerals, and coal power industries. Aspen Plus includes and large database of pure component and phase equilibrium data for conventional chemicals, electrolytes, solids, and polymers.

AspenDynamics [1] is a software from AspenTech that is able to simulate the dynamic behavior of processes. It supports concurrent process and control design.

Although tere are many process simulation software that are able to simulate either processes in steady-state or dynamic mode exist in the world, the benefit of AspenPlus and AspenDynamics is that in general an AspenPlus model can be transformed into an AspenDynamics model, so that the both the steady-state and dynamic performance can be studied enabling consideration of steady-state process performance and operability issues in parallel. Typically models made with AspenPlus can also be used in other AspenTech's software like Aspen Process Economic Analyzer that can calculate the economic (operation and investment) performance of the simulated process.

0.1.1 Objective of this report

The objective of this report is to study the possibility to use AspenDynamics as a dynamic process simulator for oxyfuel combustion processes. Especially the focus is on studying hoe existing AspenPlus models can be transformed in to AspenDynamics models. A short introduction how can this be done is given using simplified units and processes existing in a oxyfuel combustion process.

0.1.2 Scope

Not all possible models and methods of AspenPlus nor AspenDynamics are presented, only those ones needed in the overall oxyfuel process.

0.2 Model1: Simplified burner and boiler

In this section a simplified model of an oxyfuel burner and a boiler with flue gas recycle is presented in order to describe the main features of transferring an AspenPlus model into an AspenDynamics model. The AspenDynamics model is simulated with one simple test run. The very simple example is chosen because the burner and the flue gas recycling are key process steps in oxyfuel combustion processes and they are also most complicated process steps to model with AspenPlus.

First an AspenPlus model, called Model1A, is presented. This is modeled in such a way that a burner in AspenPlus would in normally be modeled. Next another AspenPlus model, called Model1B, is used to show how Model1a needs to be changed so that it can be transformed into a working AspenDynamics model. The resulting AspenDynamics model is called Model1C.

0.2.1 AspenPlus model: Model1A

The drawing of Model1A is shown in Figure 2. As can be seen, typically a burner in AspenPlus is modeled as two separate blocks, where the first block (B3 in the drawing) is a yield reactor that decomposes the solid fuel into conventional components that can be found in data bases. So the fuel is typically a nonconventional solid component that is not found directly in databases. This decomposition of a solid fuel generally consumes energy. This energy is taken from the other reactor (B1 in the drawing), where the components react which each other producing flue gases and energy. This second reactor is a RGibbs reactor, which means that it is assumed that the system reaches chemical and physical equilibrium. Certainly this equilibrium can be restricted in the RGibbs reactor with limited reactions or temperature, but for a combustion process the equilibrium assumption is decently valid. The streams entering the RGibbs reactor are the decomposed fuel (stream DECFUEL) and the mixture of oxygen (OXYGEN) and recycled flue gas (RFLUEG2), which are mixed in the mixer (B4). The stream (GASOUT) exiting the RGibbs reactor is split into two streams (2 and 3), where the gaseous components flow to the boiler (B2) and the solid components are disposed. In a real burner the solid components would be the bottom ash. Altogether the three reactors (B1,B3, B7) is one way in AspenPlus to model a burner.

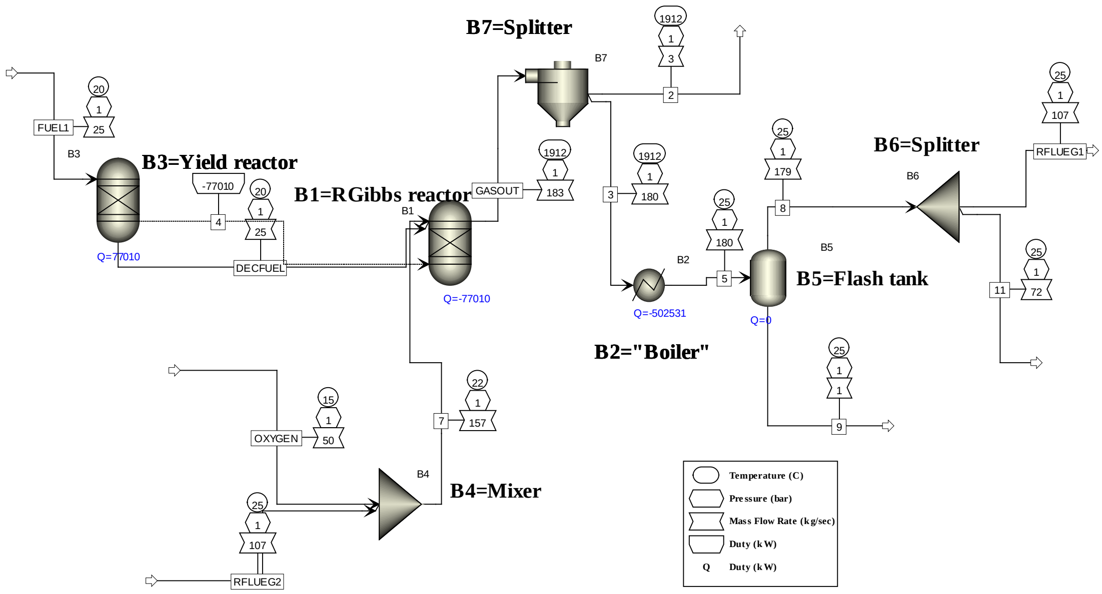

Figure 2: AspenPlus drawing of Model1A

Unit B2 is the boiler of this simple process. As can be seen in this case it is modeled as just a stream cooler, where in reality the actual boiler has many heat exchangers and connections to the turbine network. After the boiler, depending if a dry or a wet flue gas recirculation scheme is chosen, most of the water in the flue gases are flashed away in a flash tank (B5). After the flash tank most of the flue gas is recycled back to the burner (stream RFLUEG1), while the other part (stream 11) goes into the GPU process. In a real power plant, typically some kind of particle removal unit and a SO_2 removal unit exist between the boiler and the flash tank.

Typically AspenPlus models have some kind of Flowsheeting options (Calculator, Design Specification etc.) defined. In Model1A there is a Design Specification that defines that the mass flow of Stream 2 is equal to $180 kg/s$. This is controlled by varying the recycled flue gas flow (Stream RFLUEG1) from 60 to 200 kg/s. Also a Transfer block is used to copy Stream RFLUEG1 to RFLUEG2.

0.2.2 AspenPlus model: Model1B

Because the objective is to simulate the same simple process dynamically in AspenDynamics, Model1A needs to be modified. First, the reactor yield needs to be deleted, because at least in this case, the AspenModelTransformer was unsuccessful in transferring Model1A into an AspenDynamics model. Another simplifi-

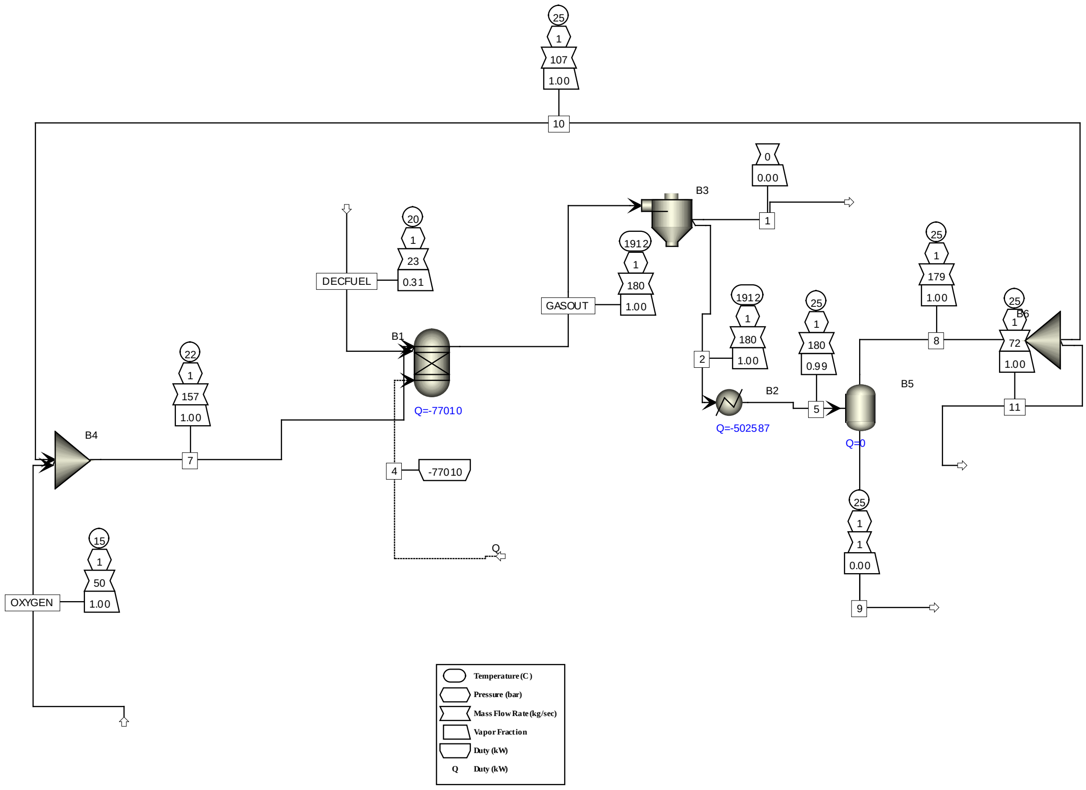

Figure 3: AspenPlus drawing of Model1B

cation needed is, that both the Transfer block and the Design Specification block of Model1A are unnecessary, because these don't work in AspenDynamics. The lack of the Transfer block is not that serious, because the AspenPlus models should work with a direct stream connection, although some changes into the Convergence settings may be needed. The deletion of the Design Specification is in that sense more serious, because if there still is a need for this specification in the dynamic model, this has to be achieved with changes in the AspenDynamics model. Figure 3 shows the AspenPlus drawing of Model1B.

0.2.3 Specifying the RGibbs reactor for dynamic simulations

There are two options for specifying the RGibbs reactor for dynamic simulations:

- Instantaneous
- PFR

The default Instantaneous reactor requires no other specifications in addition to those given for steady-state simulation. For PFR type, the reactor geometry needs to be specified.

0.2.4 Heater/Condenser

There are two options for specifying this block for dynamic simulations. The heater type is either:

- Instantaneous
- Dynamic

The instantaneous model type does not model dynamic effects. The Dynamic mode is modeled in the same way as a single side of the Heat Exchanger model: two user specified volumes are added, one for the entering stream and one for the exiting stream. Additionally for both heater types, the heat transfer option may be defined, with constant heat transfer as the default.

0.2.5 Splitter

No specification is needed or possible for either of the splitters (blocks B3 and B6) in Model1B.

0.2.6 Flash

There are three options for specifying the Flash block for dynamic simulations. The vessel type is either:

- Instantaneous
- Horizontal
- Vertical

The instantaneous model type does not model dynamic effects, except for heat transfer type. For vertical or horizontal vessels, the vessel geometry must be specified. If liquid is present at steady state, also the initial liquid volume fraction needs to be specified. Also a method of calculating the heat transfer within the vessel can be chosen. If either the horizontal or vertical vessel type is chosen, two automatic controllers for pressure or level control may be defined.

0.2.7 Mixer

There are three options for specifying the Mixer block for dynamic simulations. The vessel type is either:

- Instantaneous
- Horizontal
- Vertical

The instantaneous model type does not model dynamic effects, except for heat transfer type. For vertical or horizontal vessels, the vessel geometry must be specified. If liquid is present at steady state, also the initial liquid volume fraction needs to be specified. Also a method of calculating the heat transfer within the vessel can be chosen. If either the horizontal or vertical vessel type is chosen, an automatic controller for overall liquid level control may be defined.

0.2.8 Pressure Driven vs. Flow Driven simulation

When exporting an AspenPlus simulation to AspenDynamics, there is a choice of a Flow Driven simulation and a Pressure Driven simulation.

In an Aspen Plus steady-state simulation, the outlet stream pressures and flow rates of a block are determined from the inlet conditions to the block, and the specifications for the block. The outlet stream pressures or flow rates are not affected by the pressure in the downstream blocks. This approach is called Flow Driven simulation.

Flow driven dynamic simulations work in the same way as in Aspen Plus simulations. For each model, fixed rules are used to determine outlet flow rates and pressures, given the inlet conditions to the block. The flow driven approach is well suited to a wide range of dynamic simulation applications. In effect, this approach makes the assumption of perfect flow control. This is often a good assumption, particularly when modeling liquid only systems. For liquids, the pressure/flow dynamics are very fast, and the assumption of perfect flow control is usually accurate.

In some simulations, it is necessary to take into account the effect of downstream pressures on flow rates in streams. To account for the effect of downstream pressure, it is necessary to create a Pressure Driven simulation. In pressure driven simulations:

- The pressures of all feeds and products to the flowsheet are fixed
- Feed flow rates are not fixed

- All flow rates in the flowsheet are determined by the pressures and pressure/flow relationships around the flowsheet

The correct simulation mode to use depends on the modeling objectives. In general, if pressure is important, then Pressure Driven may be required. The correct simulation mode also depends on the type of process. Typically, simulations consisting of mostly gas or vapor phase streams will require Pressure Driven mode. Some examples of these systems are steam networks, gas networks, pressure relief systems and compressor networks. Conversely, simulations that consist of mostly liquid streams will not require Pressure Driven mode.

The control system of the simulation should also be considered. If a good pressure and good flow control exists, then Flow Driven simulation may be suitable. Also, the effect of pressure on physical properties should be considered. Pressure can have a large effect on gas stream properties, such as densities, or on reaction kinetics in some cases.

0.2.9 Dynamic specification in Model1B

In this case, all dynamic specifications are instantaneous and the dynamic modeling is flow-driven.

0.2.10 AspenDynamics model: Model1C

In AspenDynamics there are many different control schemes and different controllers available. Controllers can be used to manipulate the specified variables to obtain the required operating conditions. For example, a temperature controller can be added to manipulate the duty to keep the temperature close to a set point value. Controllers also include different options to study changes and delays in process dynamics. Also tasks can be written to force disturbances and discrete events such as unit failures. A task is a set of instructions that one can create to define a sequence of actions to take place during a dynamic simulation. For example, disturbances in feed conditions or changes to controller set points. Scripts are used to set up a simulation. A script is a set of instructions, written in Microsoft Visual Basic, to automate the setup of a simulation. A simple script is a list of assignments for parameters and variables such as default value, specification, lower and upper bounds. Scripts can also be used to control sequences of simulation runs. Also new process blocks and streams not existing in the AspenPlus model can be added.

In Model1C, which is the dynamic simulation model based on Model1B, only one simple controller is used. In this case a noise controller is used to force stochastic disturbance on the massflow of ingoming oxygen (Stream Oxygen). The Stan-

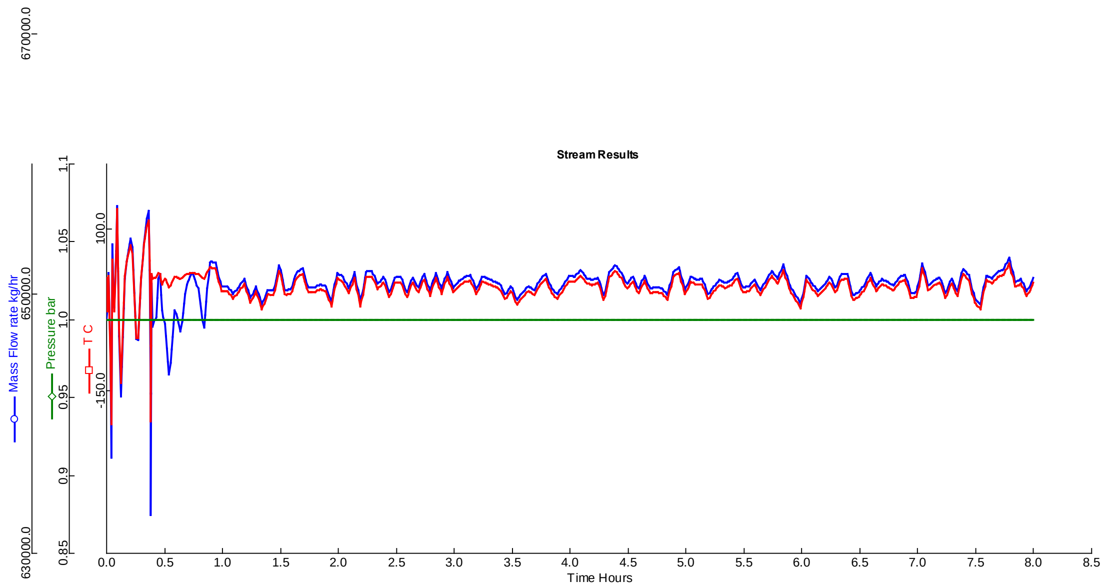

Figure 4: Temperature, pressure and massflow of Stream 5 in Model1C

dard Deviation of this noise is in this case 300 kg/hr. Figure 4 shows the results of temperature, pressure and massflow rate of Stream 5 depending on this disturbance. The simulation was running for 8 hours.

0.3 Model2: Simplified power plant with CO_2 capture and gas purification process

In this Section an example of a simplified power plant and a simplified GPU is given. First the process is modeled as a steady-state AspenPlus model, called Model2A, and then this model is transformed into an AspenDynamics model, called Model2B. This Section presents also new units introduced in the flowsheet of the simplified power plant and GPU, together with the dynamic specifications of Modela2A.

22.5 kg/s of fuel, whose analysis can be seen in Table 1, is burnt producing 200 kg/s, 441 °C and 270 bar steam. This steam that is partly reheated (180 kg/s, 382 °C and 50 bar) produces 426.1 MW electricity. The flue gas from the boiler is cooled so that most of its moisture content is condensed, and then partly (173.5 kg/s) recycled back to the boiler. The rest of the flue gas goes into the GPU where it is compressed and partly liquified. For the reason that the flue has a high portion of noncondensable gases and the GPU is so so simple, only 85% of the CO_2 entering the GPU is liquified.

0.3.1 AspenPlus model

Figure 5 shows the flowsheet of the simplified power plant and GPU.

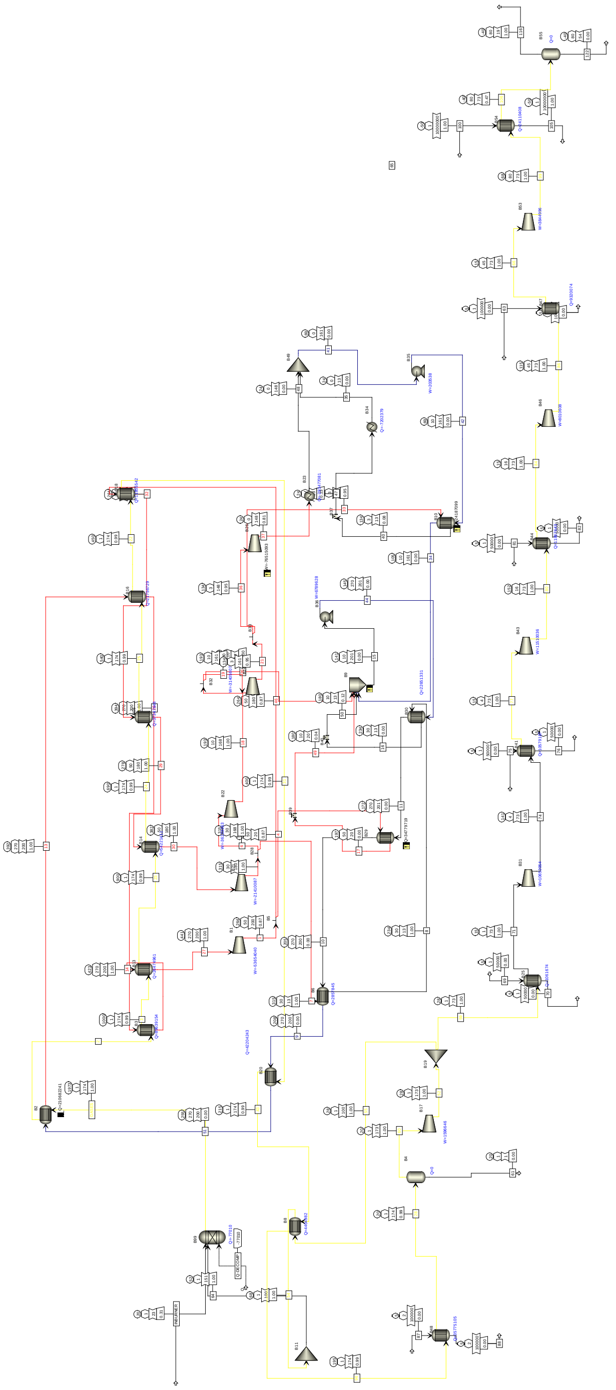

Figure 5: AspenPlus drawing of Model2A

Component	[%]
C	74
H_2	6
O_2	10
Ash	10
moisture	10

Table 1: Fuel composition

0.3.2 Compressor

A compressor can be simulated dynamically only if performance curves of the compressor are given. If only the discharge pressure is given, which is typical for general steady-state simulations, the dynamic performance of a compressor equals its steady-state performance.

0.3.3 Turbine

A turbine is like a compressor in AspenPlus, so it can be simulated dynamically only if performance curves of the turbine are given. If only the discharge pressure is given, which is typical for general steady-state simulations, the dynamic performance of a turbine equals its steady-state performance.

0.3.4 Pump

A pump is like a compressor or turbine in AspenPlus, so it can be simulated dynamically only if performance curves of the pump are given. If only the discharge pressure is given, which is typical for general steady-state simulations, the dynamic performance of a pump equals its steady-state performance.

0.3.5 HEX

There are two options for specifying the Heat Exchanger block for dynamic simulations. The model type is either:

- Instantaneous
- Dynamic

The instantaneous model type does not model dynamic effects, except for heat transfer type. For the dynamic type, both hot and cold side inlet and exit volume

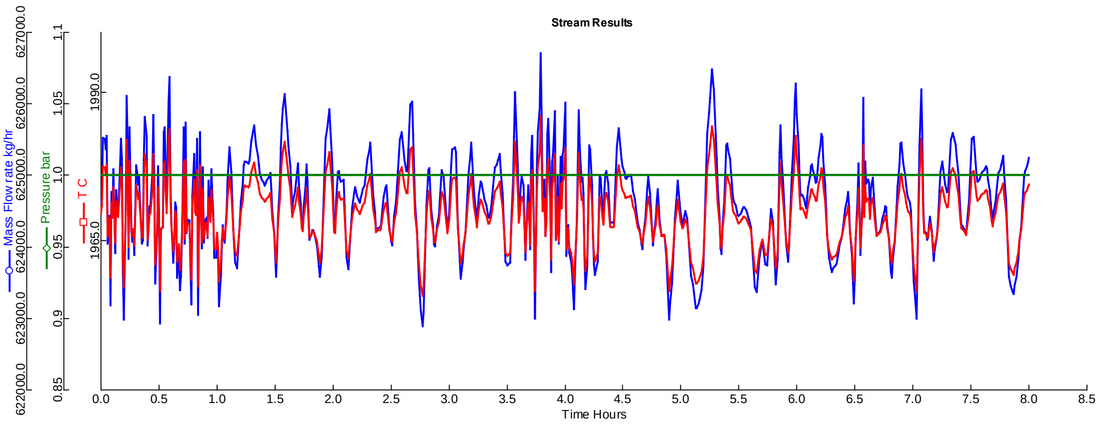

Figure 6: Temperature, pressure and massflow of Stream Gases in Model2B

need to be specified. In both model types, the pressure drop in the heat exchanger can be defined.

0.3.6 Dynamic specification in Model2A

In this case, all dynamic specifications are instantaneous except the flash tanks B4 and B55, which both have a horizontal vessel type with elliptical head having a length of 10 m and a diameter of 2 m. The dynamic modeling is flow-driven.

0.3.7 AspenDynamics model

In Model2B, which is based on the steady-state simulation model Model2A, only one simple controller is used addition to the two controllers (pressure and level) that both flash tanks B4 and B55 have. In this case a noise controller is used to force stochastic disturbance on the massflow of ingoing oxygen (Stream 62). The Standard Deviation of this noise is in this case 300 kg/hr. Figure 6 shows the results of temperature, pressure and massflow rate of Stream Gases depending on this disturbance. The simulation was running for 8 hours.

0.4 ASU

In this Section an example of a simplified Air Separation Unit (ASU) is given. First the process is modeled as a steady-state AspenPlus model, called Model3A, and then this model is transformed into an AspenDynamics model, called Model3B. This Section presents also new units introduced in the flowsheet of the ASU, together with the dynamic specifications of Modela3A.

In the steady-state model, 205 kg/s air is compressed to 5.5 $bars$ in four compression and inter-cooling stages before CO_2 and water are separated from the air in molecular sieves. This purified air is cooled in the main heat exchanger to -174 °C before entering the double column distillation. In the distillation columns most of the N_2 of the incoming air is separated from the oxygen and argon stream is lead to the power plant. In the main heat exchanger the exiting cold gases cool down the incoming air. The outgoing oxygen stream has a oxygen content of 94.7% (molar base). In the double column the high pressure column's reboiler operates as the low pressure column's condenser, so no additional heating nor cooling is needed in the double column. Because no ready model for a double column exist in AspenPlus, the model of the double column is developed as two columns, where the heat exchanger B3 operates as the reboiler of the high pressure column and the condenser of the low pressure column.

0.4.1 AspenPlus model

Figure 7 shows the flowsheet of the ASU in this case.

0.4.2 Distillation column

As new blocks not presented so far are the distillation columns B1 and B2. A lot of different dynamic simulation options are available for the columns. In this case the sump is chosen to be elliptical with a height of 100 meters with a diameter of 5 meters for both columns. An initial liquid volume level is 50%. Regarding hydraulics, simple packing with a diameter of 5 meters and the height equivalent of a theoretical plate (HETP) is 1 meter for each stage. Both the sump level and pressure controllers are applied.

0.4.3 MHEX

There are two options for specifying the Heat Exchanger block for dynamic simulations. The model type is either:

- Instantaneous
- Dynamic

The instantaneous model type does not model dynamic effects, except for heat transfer type. For dynamic type, the inlet volumes of all streams need to be defined. Important in transforming the AspenPlus model to an AspenDynamics model is that both exchanger zone profiles and stream profiles are reported in the model's results.

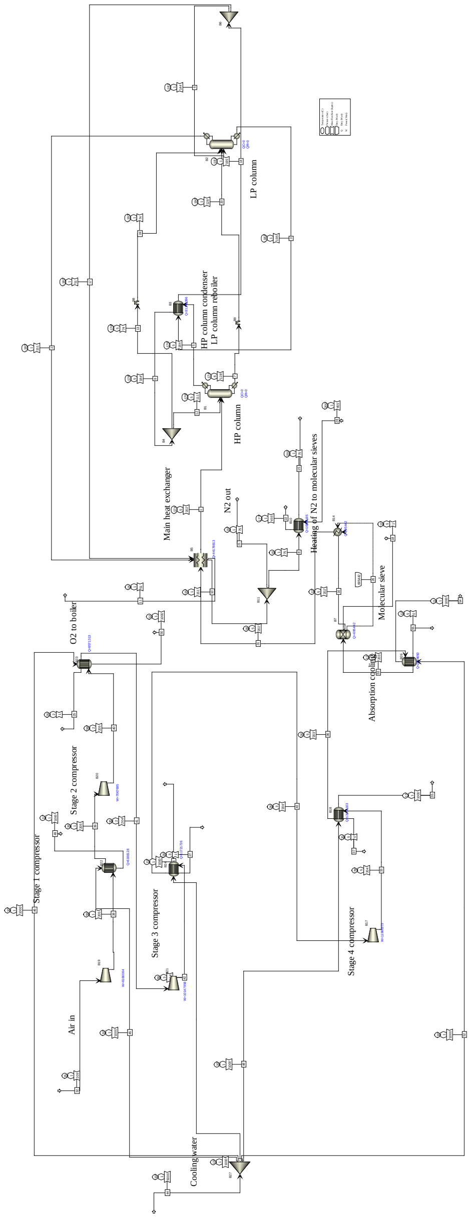

Figure 7: AspenPlus drawing of Model3A

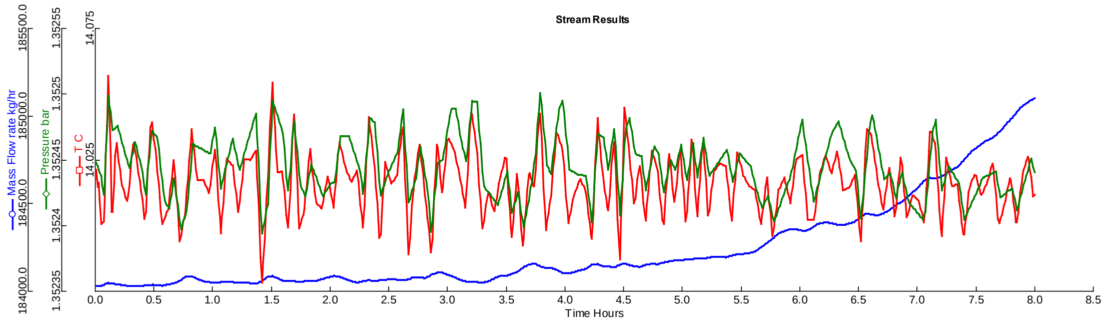

Figure 8: Temperature, pressure and massflow of oxygen flow to power plant (Stream 11 in Model3B)

0.4.4 AspenDynamics model

In Model3B, which is based on the steady-state simulation model Model3A, only one simple controller is used in addition to the two controllers (pressure at the top stage and the sump level) that both distillation columns B1 and B2 have. In this case a noise controller is used to force stochastic disturbance on the massflow of ingoing air (Stream 32). The Standard Deviation of this noise is in this case 300 kg/hr. Figure 8 shows the results of temperature, pressure and massflow rate of the outgoing oxygen flow (Stream 11) depending on this disturbance. The simulation was running for 8 hours.

0.5 Total oxyfuel process: Model4

The total oxyfuel process is a combination of the power plant and GPU process, Model2, and the ASU process, Model3. All the same process units, process parameters and process controllers are used as in the separate models. Only major difference in the combined model, Model4, is the fact that the incoming air is reduced to 185 kg/s compared to the original ASU model, Model3. Another difference is that a prefix AS is introduced to all stream and block names in the ASU if their original names were conflicting with the names of streams and blocks in the power plant and GPU model. The steady-state simulation model is called Model4A and the dynamic simulation model is called Model4B.

0.5.1 AspenPlus model

Because Model4A is just a combination of Model2A and Model3A, no diagram of it is given.

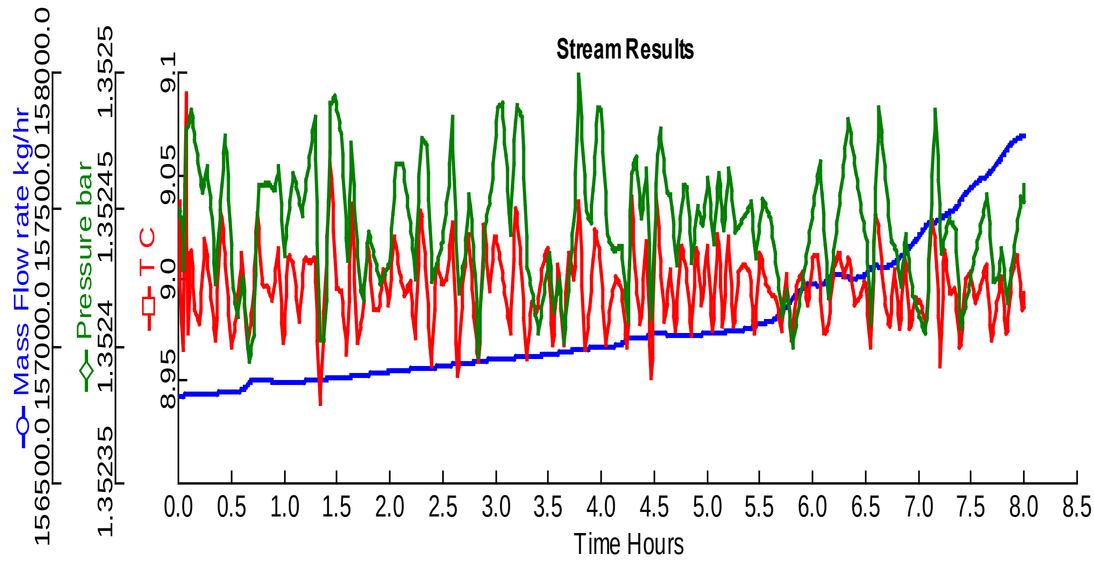

Figure 9: Temperature, pressure and massflow of the oxygen flow to power plant (Stream AS11 in Model4B)

0.5.2 AspenDynamics model

In Model4B, which is based on the steady-state simulation model Model4A, only one simple controller is used in addition to the two controllers (pressure at the top stage and the sump level) that both distillation columns ASB1 and ASB2 have and the two controllers (pressure and level) that both flash tanks B4 and B55 have. In this case a noise controller is used to force stochastic disturbance on the massflow of incoming air (Stream AS32). The Standard Deviation of this noise is in this case 300 kg/hr. Figure 9 shows the results of temperature, pressure and massflow rate of the outgoing oxygen flow (Stream AS11) depending on this disturbance. Figure 10 shows the results of temperature, pressure and massflow rate of the recycled flue gas flow (Stream 55). Figure 11 shows the results of temperature, pressure and massflow rate of the liquified CO_2 flow (Stream 122). The simulation was running for 8 hours.

0.6 Discussion and future work

In this intermediate report the objective has been to study the possibility to use AspenDynamics as a dynamic simulation tool to study the dynamic behavior of oxyfuel combustion processes. An important part has been to study how existing AspenPlus models can be transformed into AspenDynamics models. This has been accomplished by studying simplified examples of parts or the total oxyfuel

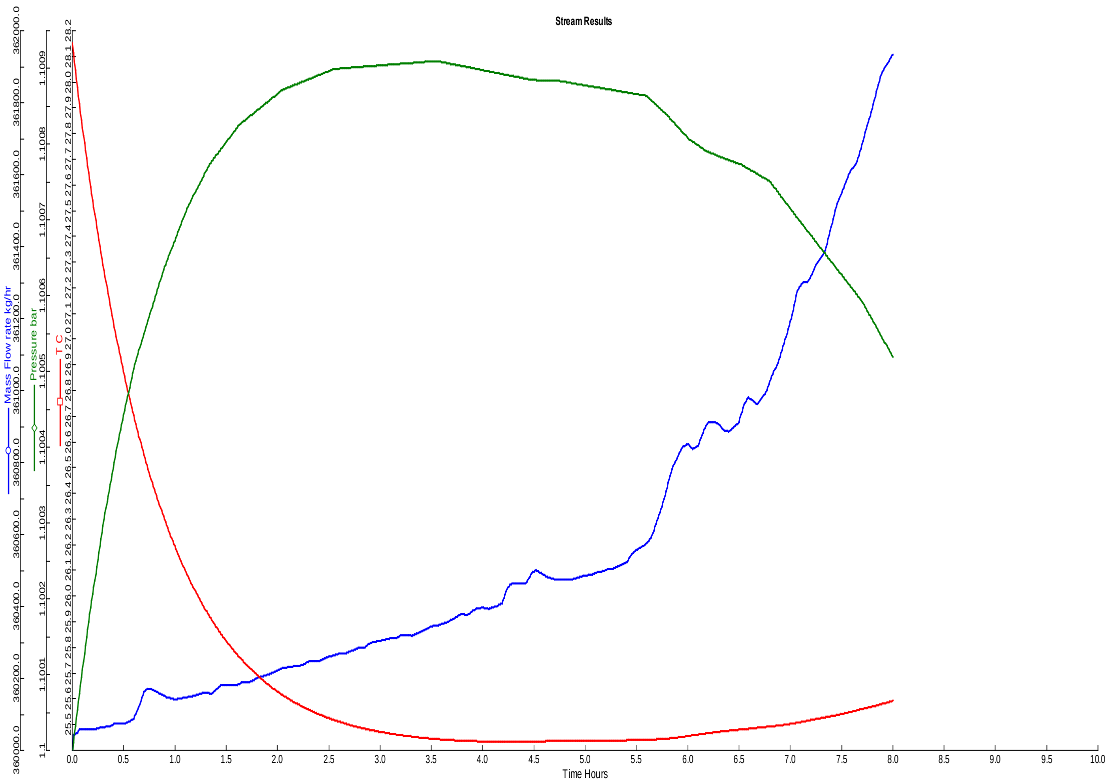

Figure 10: Temperature, pressure and massflow of the recycled flue gas flow (Stream 55 in Model4B)

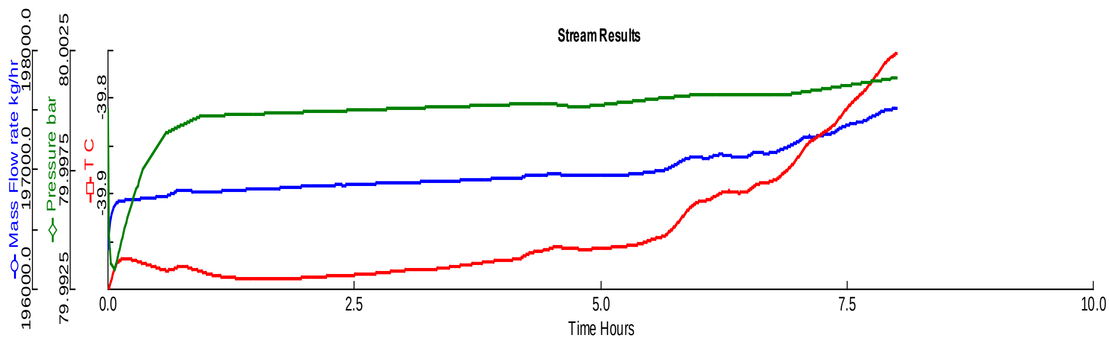

Figure 11: Temperature, pressure and massflow of the liquified CO_2 flow (Stream 122 in Model4B)

combustion process. The objective has not been to develop a fully realistic process based on a well-defined case, which is modeled in detail both in steady-state mode and dynamic mode. Nor has the objective been to study the dynamic behavior in detail and in different operating conditions or to develop a fully working control system for the process. These issues will be studied later during the project.

The first model that has been developed is the burner of the oxyfuel combustion process. This is studied because it is the burner where the biggest modifications seem to be needed in transforming an AspenPlus model into an AspenDynamics model. This burner model was then used in a model of an oxyfuel power plant having a CO_2 capture and purification unit (GPU). The third model is a model of the Air Separation Unit (ASU). This model was then integrated with the power plant and GPU process model in order to study the dynamic behavior of the total oxyfuel process.

According to the knowledge so far, it can be concluded that AspenDynamics can be used to study the dynamic behavior of oxyfuel combustion processes. The real benefit it has is that AspenPlus models can, with small modifications, be transformed into AspenDynamics models. Sometimes this can be tedious and hard to accomplish, but in general it is possible. Sometimes even though the transformation has been successful, the AspenDynamics models do not converge to a solution, but typically this problem can be solved with changing either the AspenPlus model or the AspenDynamics model.

0.6.1 Future work

In the future, the main focus will be on developing an detailed AspenPlus model of a specific case study. This model will be then transformed into a detailed AspenDynamics model, which is used to study the dynamic behavior of different operational conditions of oxyfuel combustion processes. A working control system will also be developed. Numerous tests on different operating situations will be modeled. Because carbon capture processes are expensive and not so energy-efficient, increased process integration will be applied to increase the operational efficiency. The benefits of increased integration will need to be studied with dynamic process simulations. Another important issue is that also the more rigorous pressure-driven dynamic simulations will be studied.

Bibliography

[1] Aspentech homepage. 2011.