

OPTIMIZATION OF A H₂O/CO₂ CONDENSER FOR CAPTURE OF CO₂ USING ROBUST SIMULATION SOFTWARE

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Abstract: There is rising anxiety that the increasing emission of carbon dioxide (CO₂) to the atmosphere will result in climate change with undefined consequences. This has led to development of technologies for reduction of CO₂ emissions from power stations, involving capture and sequestering of generated CO₂. New knowledge, based on both advanced combustion and gasification technologies hold promise for economically achieving CO₂ reductions through improved efficiencies. Based on judgement of the three main methods that are used for the capture of CO₂ from gas-fired power plants the author has studied Oxy-fuel cycles with internal combustion of gas using pure oxygen including the chemical looping combustion cycle.

This article provides technical research methods of capturing CO₂, which involves separating the CO₂ from the other constituents in the flue gas using a condenser. The CO₂/steam separation and condenser unit is an essential part of all oxy-fuel cycles and the CO₂ handling tools does in fact represents a considerable contribute to the total cost for such power plants. Improvements regarding cost efficiency and compactness of the CO₂/steam condenser systems is hence of vital importance if the oxy-fuel power plant concepts are going to be developed as realistic commercial alternatives. The CO₂/steam separation process does also influence the thermal efficiency and hence the operational cost of the cycle through the effect of pressure loss and through the effect of purity of re-circulated water and CO₂. The methods discussed in this paper are the CO₂/steam separation process in an oxygen fuel combustion system. The main goal is to develop a thorough understanding of the separation process at varying thermal conditions and with varying fluid compositions. A CFD tool has been used for simulation of the proposed condenser to separate H₂O and capture CO₂. It has been carried out as an optimization study that also may lead to reduced capital costs and increase the thermal efficiency of the power plants. Accurate knowledge about the thermo physical and fluid dynamic properties of CO₂/H₂O mixtures is required in order to carry out reliable process simulations and hence to optimise the condenser and the process cycles. Some experimental thermodynamic data like compressibility, dew point, density and enthalpy for CO₂/H₂O mixtures are available in previous works by the two latter authors. Fluid flow, heat transfer rate and pressure drop characteristics are studied as function of CO₂/H₂O mixture composition. Resulting velocity profile, gas/liquid ratio, degree of turbulence, two phase flow regime for H₂O/CO₂ mixtures are also presented.

1 Introduction

The aim of CO₂ capture is to generate a concentrated flow that can be fast transported to a CO₂ storage site. CO₂ capture and storage is most appropriate to big, centralized sources similar to power plants and huge industries. Total efficiency of power plant or industries decreases due to energy consumption to run CO₂ capture systems, leading to increased fuels, solid wastes and environmental pollutants relative to the same type of base plant without capture.

Though, as more efficient plants with capture become available and replace many of the older less efficient plants now in service, the net impacts will be compatible with clean air emission goals for fossil fuel use.

At present, CO₂ is routinely separated at some large industrial plants such as natural gas processing and ammonia production facilities, although these plants remove CO₂ to meet process demands and not for storage. CO₂ capture also as been applied to several small power plants. However, there have been no applications at large-scale power plants of several hundred megawatts, the major source of current and projected CO₂ emissions.

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There are three main approaches to CO₂ capture, for industrial and power plant applications. *Post-combustion* systems separate CO₂ from the flue gases produced by combustion of a primary fuel (coal, natural gas, oil or biomass) in air. *Oxy-fuel combustion* uses oxygen instead of air for combustion, producing a flue gas that is mainly H₂O and CO₂ and which is readily captured. This is an option still under development. *Pre-combustion* systems process the primary fuel in a reactor to produce separate streams of CO₂ for storage and H₂ which is used as a fuel. The monitoring, risk and legal aspects associated with CO₂ capture systems appear to present no new challenges, as they are all elements of long-standing health, safety and environmental control practice in industry. The following part 1 has been written base on IPCC reports in general to better perceive of process.

Based on the IPCC report [2], " industrial CO₂ capture systems can reduce CO₂ emissions from power plants by 80-90% kWh⁻¹ (85- 95% capture efficiency) at now. Across all plant types the cost of electricity production (COE) increases by 12-36 US\$ MWh⁻¹(US\$ 0.012-0.036 kWh⁻¹) over a similar type of plant without capture, corresponding to a 40-85% increase for a supercritical pulverized coal (PC) plant, 35-70% for a natural gas combined cycle (NGCC) plant and 20-55% for an integrated gasification combined cycle (IGCC) plant using bituminous coal. Overall the COE for fossil fuel plants with capture, ranges from 43-86 US\$ MWh⁻¹, with the cost per tonne of CO₂ ranging from 11- 57 US\$/tCO₂ captured or 13-74 US\$/tCO₂ avoided (depending on plant type, size, fuel type and a host of other factors). These costs include CO₂ compression but not additional transport and storage costs. NGCC systems typically have a lower COE than new PC and IGCC plants (with or without capture) for gas prices below about 4 US\$ GJ⁻¹.

Most researches specify that IGCC plants are slightly more costly without capture and slightly less costly with capture than similarly sized PC plants, but the differences in cost for plants with CO₂ capture can vary with coal type and other local factors. The lowest CO₂ capture costs (averaging about 12 US\$/t CO₂ captured or 15 US\$/tCO₂ avoided) were found for industrial processes such as hydrogen production plants that produce concentrated CO₂ streams as part of the current production process; such industrial processes may represent some of the earliest opportunities for CO₂ Capture and Storage (CCS). Generally, CO₂ capture costs are highly dependent upon technical, economic and financial factors related to the design and operation of the production process or power system of interest, as well as the design and operation of the CO₂ capture technology employed.

Modified methods of CO₂ capture, combined with improved power systems and industrial process designs, can significantly reduce CO₂ capture costs and associated energy requirements. While there is considerable uncertainty about the magnitude and timing of future cost reductions, IPCC assessment suggests that improvements of commercial technologies can reduce CO₂ capture costs by at least 20-30% over the next decade, while new technologies under development promise more substantial cost reductions.

1.1 General remarks of emissions from capture systems

CO₂ capture equipped plants would generate a flow of concentrated CO₂ for storage, plus in most cases a flue gas or vent gas emitted to the atmosphere together with some liquid wastes. In some cases solid wastes will also be produced. The captured CO₂ flow may contain impurities which would have practical impacts on CO₂ transport and storage systems and also potential health, safety and environmental impacts. The types and concentrations of impurities depend on the type of capture process, as shown in Table 1, and detailed plant design. The major impurities in CO₂ are well known but there is little published information on the fate of any trace impurities in the feed gas such as heavy metals. If substances are captured along with the CO₂ then their net emissions to the atmosphere will be reduced, but impurities in the CO₂ may result in environmental impacts at the storage site.

Stored CO₂ from most capture processes contains moisture, which has to be removed to avoid corrosion and hydrate formation during transportation. This can be done using conventional costs of CO₂ capture plants.

	SO ₂	NO	H ₂ S	H ₂	CO	CH ₄	N ₂ /Ar/O ₂	Total
Coal fired plants								
Post combustion capture	<0.01	<0.01	0	0	0	0	0.01	0.01
Pre combustion capture	0	0	0.01-0.6	0.8-2	0.03-0.4	0.01	0.03-0.6	2.1-2.7
Oxy fuel	0.5	0.01	0	0	0	0	3.7	4.2
Gas fired plants								
Post combustion capture	<0.01	<0.01	0	0	0	0	0.01	0.01
Pre combustion capture	0	0	0.01	1	0.04	2	1.3	4.4
Oxy fuel	<0.01	<0.01	0	0	0	0	4.1	4.1

Table 1. Concentrations of impurities in dried CO₂, % by volume (Source data: IEA GHG, 2003; IEA GHG, 2004; IEA GHG, 2005).

The CO₂-rich gas obtained from oxy-fuel processes is including of oxygen, nitrogen, argon, sulphur and nitrogen oxides and various other impurities. This gas will normally be compressed and fed to a cryogenic purification process to reduce the impurities concentrations to the levels required to avoid two-phase flow

conditions in the transportation pipelines. A 99.99% purity could be obtained by including distillation in the cryogenic separation unit. Otherwise, the sulphur and nitrogen oxides could be left in the CO₂ fed to storage in circumstances where that is environmentally acceptable as described above for pre-combustion capture and when the total amount of all impurities left in the CO₂ is low enough to avoid two-phase flow conditions in transportation pipelines.

Power plants with CO₂ capture would emit a CO₂-depleted flue gas to the atmosphere. The concentrations of most harmful substances in the flue gas would be similar to or lower than in the flue gas from plants without CO₂ capture, because CO₂ capture processes inherently remove some impurities and some other impurities have to be removed upstream to enable the CO₂ capture process to operate effectively.

According to table 1: a. The SO₂ concentration for oxy-fuel and the maximum H₂S concentration for pre-combustion capture are for cases where these impurities are deliberately left in the CO₂, to reduce the costs of capture. The concentrations shown in the table are based on use of coal with a sulphur content of 0.86%. The concentrations would be directly proportional to the fuel sulphur content.

b. The oxy-fuel case includes cryogenic purification of the CO₂ to separate some of the N₂, Ar, O₂ and NO_x. Removal of this unit would increase impurity concentrations but reduce costs.

c. For all technologies, the impurity concentrations shown in the table could be reduced at higher capture costs.

1.2 Oxy-fuel combustion capture systems

nitrogen from the flue gas in the oxy-fuel combustion process is eliminated by combusting a hydrocarbon or carbonaceous fuel in either pure oxygen or a mixture of pure oxygen and a CO₂ rich recycled flue gas (carbonaceous fuels include biomass).

Fuel with pure oxygen combustion's has a temperature of about 3500°C which is far too high for typical power plant materials. The combustion temperature is limited to about 1300-1400°C in a typical gas turbine cycle and to about 1900°C in an oxy-fuel coal-fired boiler using current technology. The combustion temperature is controlled by the proportion of flue gas and gaseous or liquid-water recycled back to the combustion chamber.

The combustion products (or flue gas) consist mainly of carbon dioxide and water vapour together with excess oxygen required to ensure complete combustion of the fuel. It will also contain any other components in the fuel, any diluents in the oxygen stream supplied, and any inerts in the fuel and from air leakage into the system from the atmosphere. The net flue gas, after cooling to condense water vapour, contains from about 80-98% CO₂ depending on the fuel used and the particular oxy-fuel combustion process. This concentrated CO₂ stream can be compressed, dried and further purified before delivery into a pipeline for storage. The CO₂ capture efficiency is very close to 100% in oxy-fuel combustion capture systems. Impurities in the CO₂ are gas components such as SO_x, NO_x, HCl and Hg derived from the fuel used, and the inert gas components, such as nitrogen, argon and oxygen, derived from the oxygen feed or air leakage into the system. The CO₂ is transported by pipeline as a dense supercritical phase. Inert gases must be reduced to a low concentration to avoid two phase flow conditions developing in the pipeline systems.

The acid gas components may need to be removed to comply with legislation covering co-disposal of toxic or hazardous waste or to avoid operations or environmental problems with disposal in deep saline reservoirs, hydrocarbon formations or in the ocean. The carbon dioxide must also be dried to prevent water condensation and corrosion in pipelines and allow use of conventional carbon-steel materials.

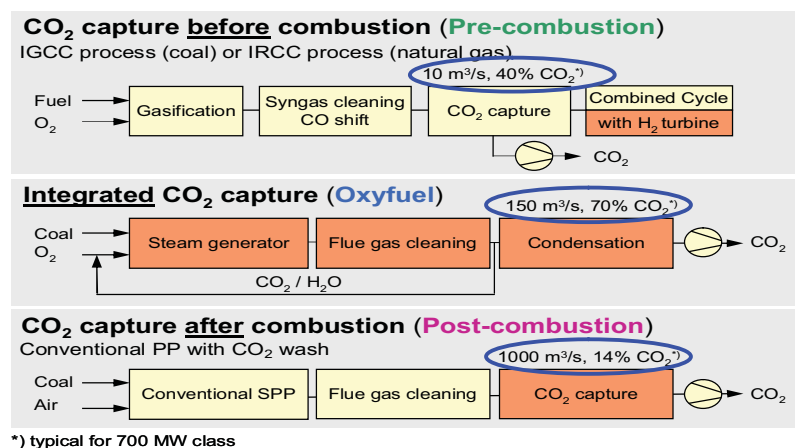


Figure 1. Competing approaches for CO₂ Capture. [1]

Figure 1 shows the comparison of three different kinds of combustion in relation with dioxide carbon capturing. High Pressure with High CO₂ concentration in pre combustion, Low Pressure and High CO₂ concentration in

Oxy fuel and so Low Pressure with High CO₂ concentration in post combustion system. Oxy-Fuel can produce a high CO₂ concentration that reduces energy requirements for capture and recovery.

1.3 Oxy-fuel direct heating - gas turbine cycle

Oxy-fuel combustion takes place in a pressurized CO₂-rich re circulating stream in a modified gas turbine. The hot gas is expanded in the turbine producing power. The turbine exhaust is cooled to provide heat for a steam cycle and water vapour is condensed by further cooling. The CO₂-rich gas is compressed in the compressor section. The net CO₂-rich combustion product is removed from the system. Only natural gas, light hydrocarbons and syngas (CO + H₂) can be used as fuel.

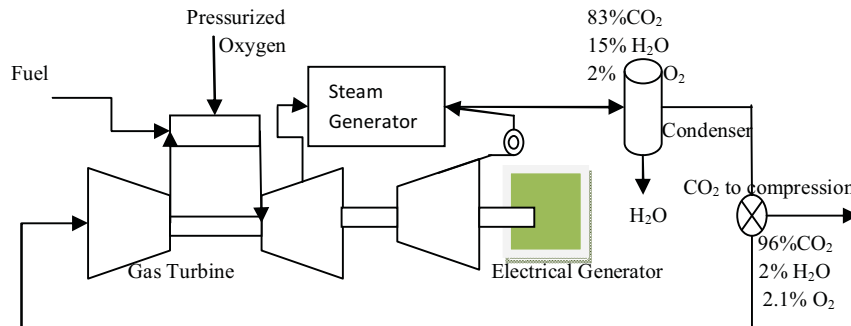


Figure 2 Principle of the oxy-fuel gas turbine combined cycle. Exhaust gas is recycled, compressed and used in the combustion chamber to control the temperature entering the turbine.

Figure 2 shows how a gas turbine can be adapted to run with oxy-fuel firing using CO₂ as a working fluid. Exhaust gas leaving the heat recovery steam generator is cooled to condense water. The net CO₂ product is removed and the remaining gas is recycled to the compressor. Suitable fuels are natural gas, light to medium hydrocarbons or (H₂ + CO) syngas, which could be derived from coal. The use of CO₂ as the working fluid in the turbine will necessitate a complete redesign of the gas turbine.

In existing gas turbines the molecular weight of the gases in the compressor and turbine are close to that of air (28.8). In the case of oxy-fuel combustion with CO₂-recycle the compressor fluid molecular weight is about 43 and about 40 in the turbine. The change in working fluid from air to a CO₂-rich gas results in a number of changes in properties that are of importance for the design of the compressor, combustor and the hot gas path including the turbine:

- The speed of sound is 80% of air;
- The gas density is 50% higher than air;
- The specific heat ratio is lower than air resulting in a lower temperature change on adiabatic compression or expansion.

An oxy-fuel gas turbine in a combined cycle has a higher optimal pressure ratio, typically 30 to 35 compared to 15 to 18 used with air in a combined cycle system. With the highest turbine inlet temperature consistent with material limitations, the rather high-pressure ratio results in an exhaust gas temperature of about 600°C, which is optimal for the steam cycle.

These changes in the fundamental properties of the working fluid will have a significant impact on gas turbine components, requiring completely new designs of compressors, combustors (to account for aerodynamic changes and acoustic feedbacks) and hot gas path (O₂ partial pressure must be low in oxy-fuel systems but it is also important to avoid reducing conditions for the materials of the turbine or the change to materials allowing much lower O₂ partial pressures).

1.4 CO₂ properties

At normal temperature and pressure, carbon dioxide is a gas. The physical state of CO₂ varies with temperature and pressure as shown in Figure 3 at low temperatures CO₂ is a solid; on warming, if the pressure is below 5.1 bar, the solid will sublime directly into the vapour state. At intermediate temperatures (between -56.5°C, the temperature of the triple point, and 31.1°C, the critical point), CO₂ may be turned from a vapour into a liquid by compressing it to the corresponding liquefaction pressure (and removing the heat produced). At temperatures higher than 31.1°C (if the pressure is greater than 73.9 bar, the pressure at the critical point), CO₂ is said to be in a supercritical state where it behaves as a gas; indeed under high pressure, the density of the gas can be very large, approaching or even exceeding the density of liquid water. This is an important aspect of CO₂'s behaviour and is particularly relevant for its storage.

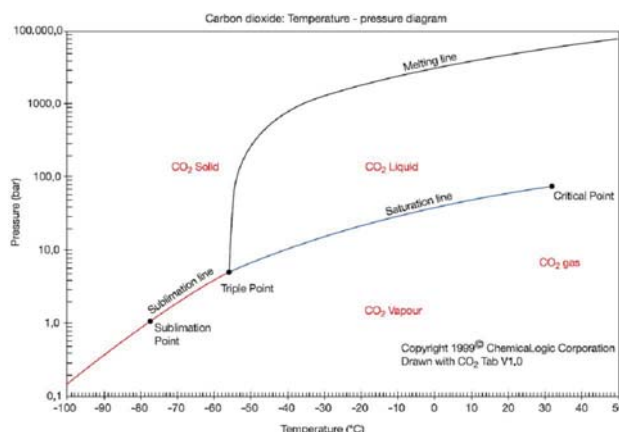


Figure 3 Phase diagram for CO₂. Copyright © 1999 ChemicaLogic Corporation, 99 South Bedford Street, Suite 207, Burlington, MA 01803 USA. All rights reserved. [2]

Heat is released or absorbed in each of the phase changes across the solid-gas, solid-liquid and liquid-gas boundaries (see Figure 3). However, the phase changes from the supercritical condition to liquid or from supercritical to gas do not require or release heat. This property is useful for the design of CO₂ compression facilities since, if this can be exploited, it avoids the need to handle the heat associated with the liquid-gas phase change''.

Property Value	
Molecular weight	44.01
Critical temperature	31.1 °C
Critical pressure	73.9 bar
Critical	467 kg m ⁻³
Triple point temperature	-56.5 °C
Triple point pressure	5.18 bar
Boiling (sublimation) point (1.013 bar)	-78.5 °C
<i>Gas Phase</i>	<i>Gas Phase</i>
Gas density (1.013 bar at boiling point)	2.814 kg m ⁻³
Gas density (@ STP)	1.976 kg m ⁻³
Specific volume (@ STP)	0.506 m ³ kg ⁻¹
Cp (@ STP)	0.0364 kJ (mol ⁻¹ K ⁻¹)
Cv (@ STP)	0.0278 kJ (mol ⁻¹ K ⁻¹)
Cp/Cv (@ STP)	1.308
Viscosity (@ STP)	13.72 μN.s m ⁻² (or μPa.s)
Thermal conductivity (@ STP)	14.65 mW (m K ⁻¹)
Solubility in water (@ STP)	1.716 vol vol ⁻¹
Enthalpy (@ STP)	21.34 kJ mol ⁻¹
Entropy (@ STP)	117.2 J mol K ⁻¹
Entropy of formation	213.8 J mol K ⁻¹
<i>Liquid Phase</i>	<i>Liquid Phase</i>
Vapour pressure (at 20 °C)	58.5 bar
Liquid density (at -20 °C and 19.7 bar)	1032 kg m ⁻³
Viscosity (@ STP)	99 μN.s m ⁻² (or μPa.s)
<i>Solid Phase</i>	<i>Solid Phase</i>
Density of carbon dioxide snow at freezing point	1562 kg m ⁻³
Latent heat of vaporisation (1.013 bar at sublimation point)	571.1 kJ kg ⁻¹

Table 1. Physical properties of CO₂. [2]

2 Proposed H₂O/CO₂ condenser simulation

In order to find a suitable design for the H₂O/CO₂ condenser, different concept layouts of condensers have been considered during this work. Figure 4 shows the geometry of proposed H₂O/CO₂ condenser. More detail information could be found in the next report of the authors that will be published later.

In figure 3, flow enters from one inlet at the left, but can leave the valve through two outlets at the top and bottom in gas and fluid mode. The choice of outlet depends on the position of the gas and fluid valve. In this model, two valves are located for flue gas input. This will be used to adjust the flow path through the outlets, depending on the position of the valves.

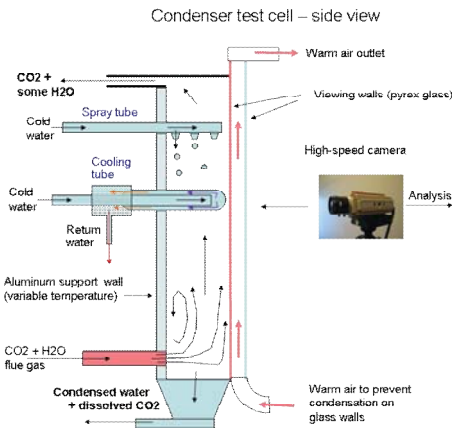


Figure 4: Depiction of the geometry of proposed H₂O/CO₂ condenser.

Flue gases from a combustion power plant are usually above 100°C, which means that they need to be cooled down to the temperature levels required for the absorption process and with removal of other impurities as well. This can be done in a condenser with direct water contact, which also acts as a flue gas wash with additional removal of fine particulates and water content removing. Flue gases from natural gas combustion will normally only contain steam and NO_x.

2.1 Model Geometry in COMSOL

In the COMSOL environment a powerful Multiphysics software, for modelling and solving a variety of problems based on partial differential equations (PDEs) has been used in this study. With this software authors easily extend physics of condenser model into multiphysics models that solved coupled physics phenomena and do so simultaneously. Simulation of the condenser involved fluid dynamics, heat transfer and fluid thermal interactions. It is possible to build models by defining the relevant physical quantities such as material properties, loads, constraints, sources, and fluxes rather than by defining the underlying equations. It can apply these variables, expressions, or numbers directly to solid domains, boundaries, edges, and points independently of the computational mesh. COMSOL Multiphysics then internally compiles a set of PDEs representing the entire model. COMSOL Multiphysics is a standalone product with flexible graphical user interface, or it may work by script programming in the COMSOL Script language or even in the MATLAB language. Figure 5 shows an outline of the condenser geometry visualized with COMSOL. Units are in meters.

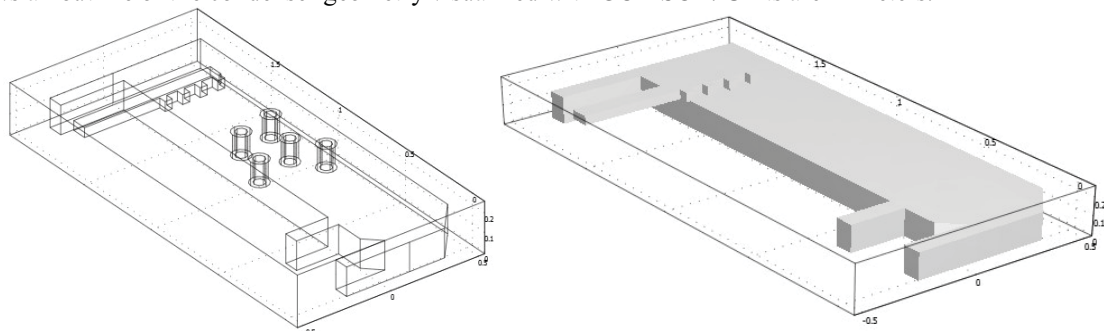


Figure 5. Model geometry and meshed geometry in COMSOL software

The domain of water tube has the following fluid parameters: viscosity $1e-4$ N·s/m² and pressure 101.325 Pa and density in 1000kg/m³. The inlet flue gases parameters are: viscosity $7e-8$ N·s/m² and pressure 150.000 Pa and density 1 kg/m³. Outlet pressure is assumed to be 101.325 Pa. Water inlet velocity is 1 m/s and inlet velocity for CO₂ is 3m/s. Boundary conditions are modelled in the following way: At the inlet, the model uses a fully developed normal flow pressure, laminar flow. The pressure is set to 150,000 Pa. At the outlets, a neutral boundary condition states that the normal component of the stress tensor is zero: The input flue gas composition in percentage is for CO₂ = 83, H₂O = 15, O₂ = 2. The temperature is 50 (°C), mass flow is 8.2 (kg/s), and pressure 1 (bar). A transient solution has been used in times from 0:0.02:3 and 3:0.2:10 min, with relative tolerance to 0.001, and absolute tolerance to 0.0001. Maximum element size for mesh considered to 0.0004 and element growth rate to 1.5. Triangular mesh with 827,234 triangles was made to do the higher degree simulation.

2.2 Results and discussion

A literature survey was performed in order to find accurate experimental data for CO₂/H₂O-mixtures. With this data the fluidynamic property package Multiphysics was validated, and different equations of state and transport property models, for pressure and temperature conditions encountered in the O₂/CO₂ gas turbine cycle, were investigated. With the condenser, velocity simulated in order to predict the importance of choosing the right method for calculating the fluid and thermodynamic properties.

Data for pure CO₂ was collected from [2 and 4] and compared with data calculated from COMSOL and MATLAB.

According to authors last proposed model [4] results improve in 2D and extend to 3D. A proposed model of the H₂O/CO₂ condenser presented in figure 4 is simulated using COMSOL multi physics software. The mesh generated of the model is illustrated in figure 5. It is based on a refined triangular mesh. Simulation results with focus on velocity field are shown in figure 6. The figures show a turbulence regime in the sprayer and condenser pipes. In the condenser tank the flow is predominantly laminar. Iteration in three dimensional simulations is about 3500 iterations and is higher than of predicted and expected values. It is shown in figure 7. Figure 8 showed the velocity field between the condenser pipes. It will be necessary to carry out studies on the velocity field around the various elements of the condenser to optimize of model in a subsequent designing step. Simulations showed generally low velocity fluctuations along the condenser and around the pipes.

The simulation results are in accordance with previous results. Because of the use of different equation to simulate of models, increasing the velocity leads to a greater difference between time dependent calculations and transient calculations, while increased water content has significant influence on the simulation accuracy. In terms of computational efforts, the simulation time increases somewhat when 3D is used instead of 2D.

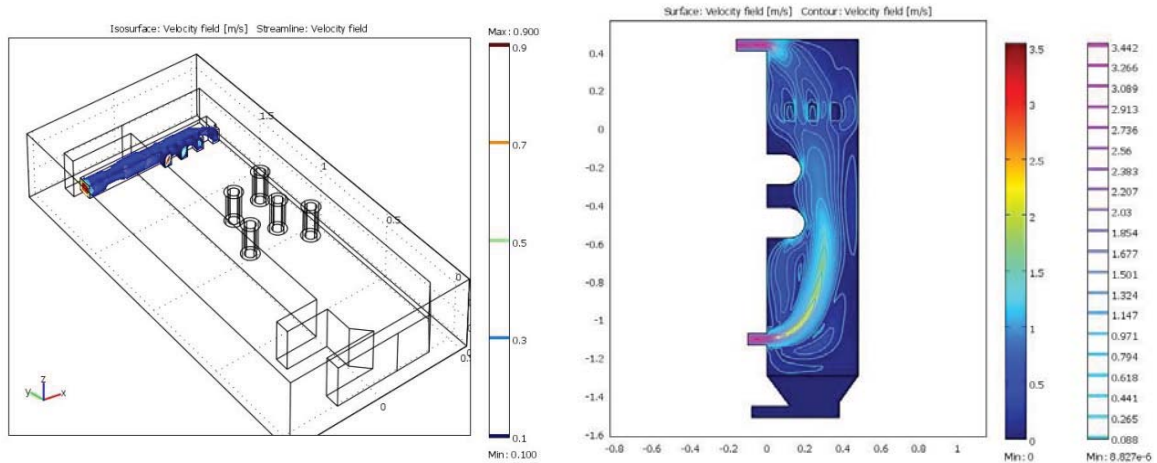


Figure 6. Velocity field in sprayer and condenser

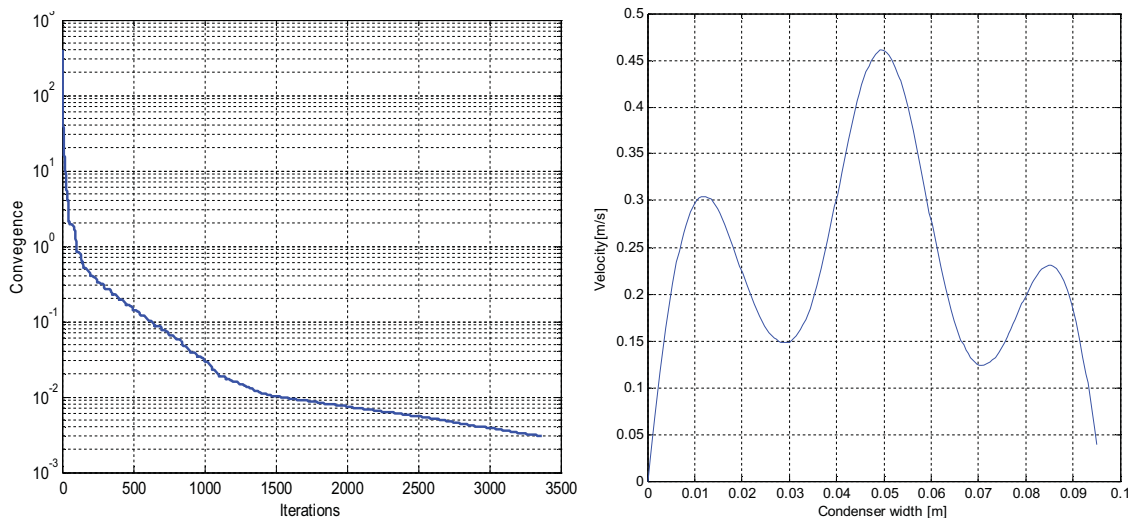


Figure 7. Convergence of simulation

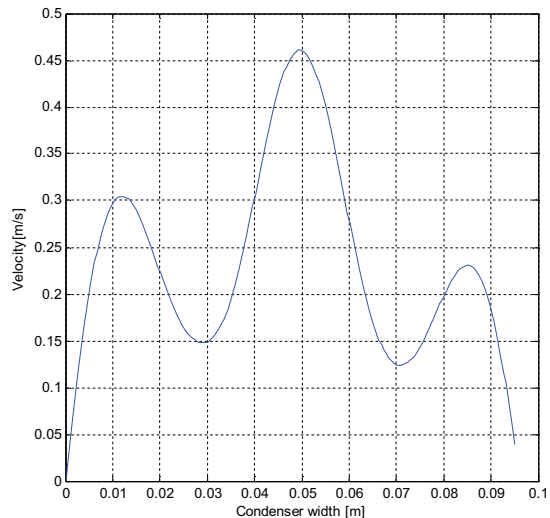


Figure 8. Velocity field between condenser tubes of figure 6.

	Flue gas (in)	Flue gas (out)	Cooler (in)	Cooler (out)
Composition (%)	CO ₂ = 83, H ₂ O = 15, O ₂ = 2	CO ₂ = 97.8, H ₂ O = 1.2, O ₂ = 1	water = 100	water = 100, CO ₂ = 0.02
Temperature (°C)	50	27.8	25	51
Velocity m/s	3	2.99	1.7	1.5
Mass flow (kg/s)	8.7	8.5	9.5	9.7

Table 2. Simulation result in brief

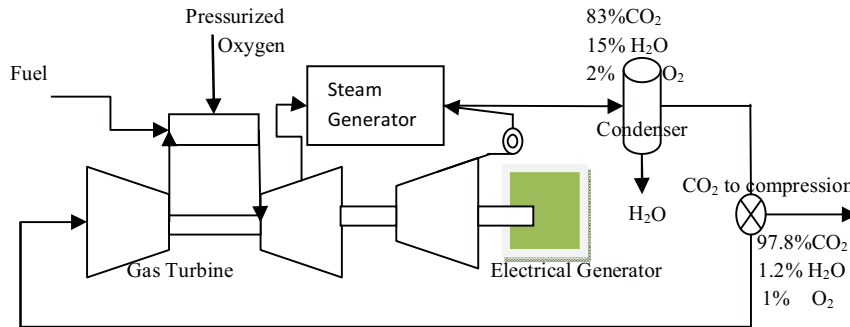


Figure 9. Exhaust gas results of simulation.

Table 2 describes concluded results which are simulated to investigate the influence the sprayer and condenser tubes have on performance calculation. Without condenser the compressor working fluid consists of 83% CO₂, 15% H₂O and 2% O₂. The compressor inlet temperature is 298 K. After using of proposed condenser, simulation results showed in outlet is consists of 97.8% CO₂, 1.2% H₂O and 1% O₂. The models are coherent with changed inlet conditions for working fluid composition and condenser outlet velocity and pressure. See figure 9. Simulation results in 3D and 2D model are in good accordance with author's previous results in [4].

3 Conclusion

The purpose of CO₂ capture is to produce a concentrated stream that can be readily transported to a CO₂ storage site. CO₂ capture and storage is most applicable to large, centralized sources like power plants and large industries.

An H₂O/CO₂ condenser intended for oxy fuel combustion system with two phase flow simulated. Inlet CO₂ was 83% with 15% water and 2% O₂ and 3m/s velocity. COMSOL multiphysics software was used for numerical simulation. The simulations showed that the outlet CO₂ concentration is 97.8% with 2.99 m/s flow velocity. Table 2 shows the simulation result in brief.

The proposed H₂O/CO₂ condenser model can satisfy the oxyfuel combustion system in power plants to capture of CO₂ with higher efficiency. As CO₂ capture increases the final cost of electricity due to higher energy consumption, it seems this model can be more economic than other designed CO₂ capture systems.

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