Twelfth Annual Conference on
Carbon Capture, Utilization & Sequestration

Oxycombustion

Kinetic Simulation of a 100kWth Oxy-Combustor using Aspen Plus

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Aim

Study the oxy-combustion process, co-firing blends of coal and biomass, through a rate-based simulation model.

The validated model will be used as a tool to select future test parameters

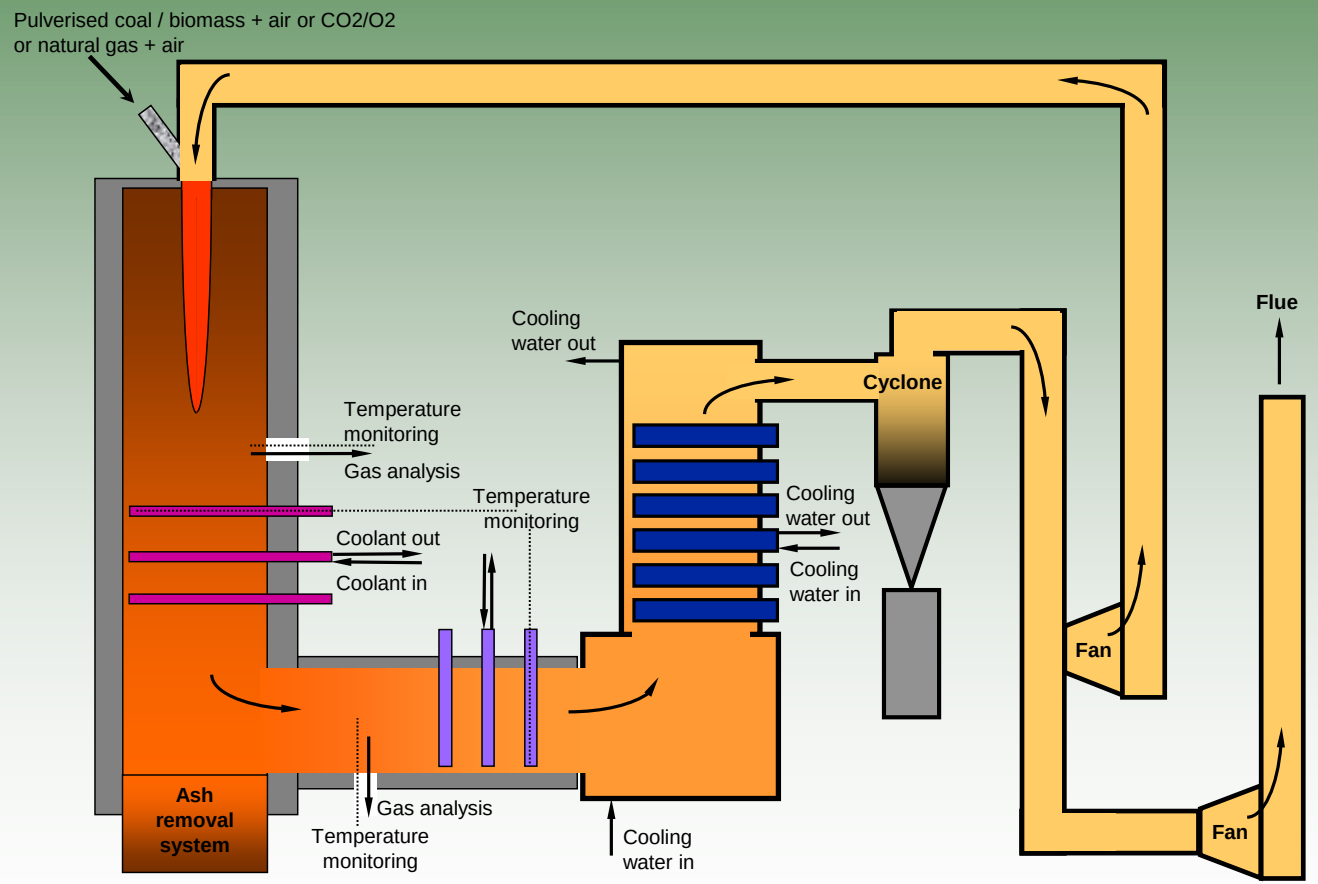
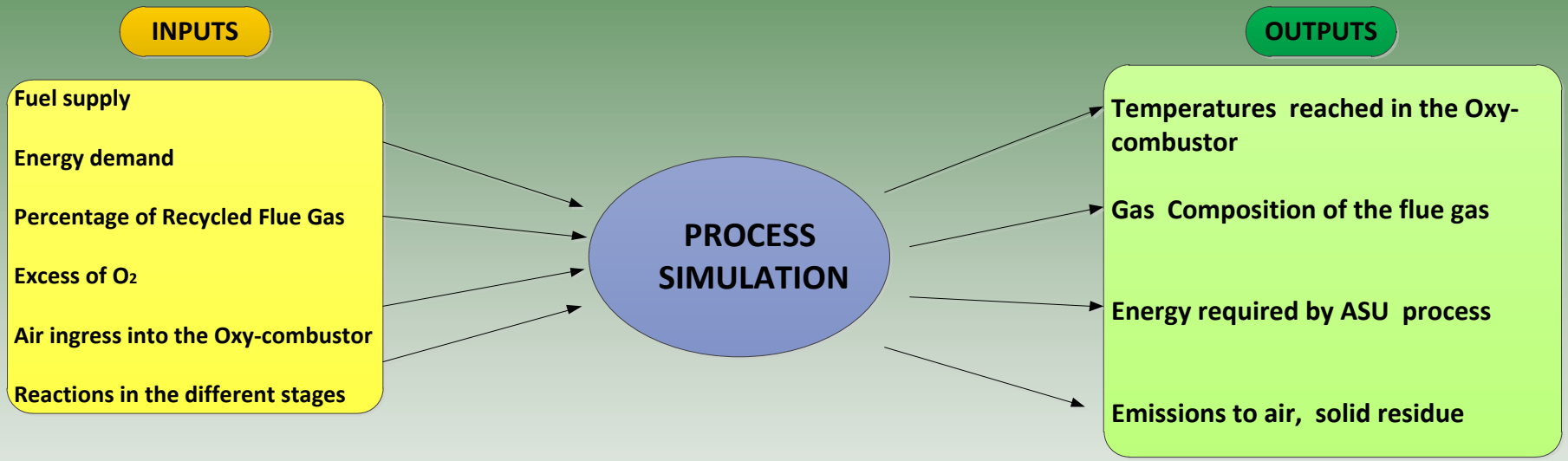


Diagram of 100kWth Multi-fuel Oxy-Combustor at CERT

Simulation Process
BASICS



Limitations of Aspen Plus

- ✓ Prediction of adiabatic flame temperature (without considering composition of the gas for the heat transfer)
- ✓ Solid residue same composition as ash defined as input (inability to simulate reaction involving solid phase)

Simulations using Aspen Plus®

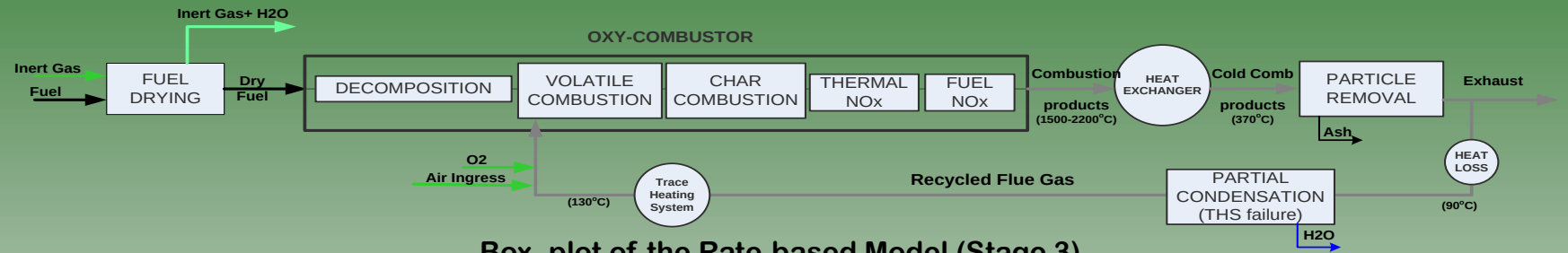
STAGES

	STAGE 1 Air-firing case	STAGE 2 Oxy-firing case with wet recirculation, heat loss and air leakage	STAGE 3 Oxy-firing case with partial condensation in RFG, heat loss and air leakage	STAGE 4 Oxy-firing case with dry recirculation, heat loss, air leakage	STAGE 5 Air-firing case with power generation unit	STAGE 6 Oxy-firing case with dry recirculation, heat loss, air leakage, ASU and power generation unit
AIR/ OXY-FIRING	Air -firing	Oxy -firing	Oxy -firing	Oxy -firing	Air -firing	Oxy -firing
RFG (%)	--	55, 60, 65, 70	55, 60, 65, 70	55, 60, 65	--	55, 60, 65
O_2 Exc (%) (v/v)	21	0,5,10	0,5	0,5	21	0,5
T_{RFG} (ºC)	--	130	75,90	130	--	130-200
Air Leakage (% of Total Gas fed)	--	1.7	0, 2, 10, 18	10	--	10
Fuel	Coal	Coal (El Cerrejon, Daw Mill), Biomass(Cereal Co-Product, Miscanthus), blends of coal and biomass (75/25; 50/50; 25/75)	Daw Mill coal, Cereal Co-Product biomass, blends of coal and biomass (75/25; 50/50; 25/75)	El Cerrejon coal, Cereal Co-Product biomass, blends of coal and biomass (75/25; 50/50; 25/75)	Coal	El Cerrejon coal, Cereal Co-Product biomass, blends of coal and biomass (75/25; 50/50; 25/75)
RFG Purification	Particle removal	Particle removal	Particle removal	Particle removal, acid species and water vapour condensation	Particle removal, acid species and water vapour condensation	Particle removal, acid species and water vapour condensation

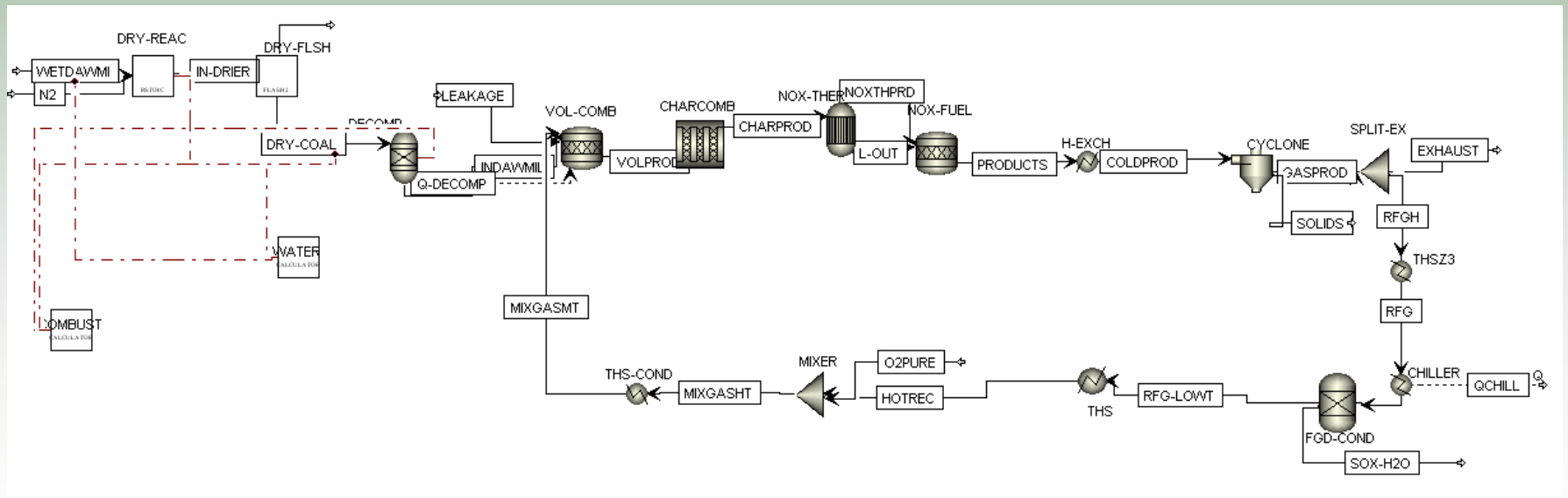
- ✓ Establish reference cases (Stages 1 and 5)
- ✓ Validation of the model by applying similar conditions to experiments (Stage 3)
- ✓ Simulations with condenser implemented to include dry RFG (Stage 4)
- ✓ Simulation of the entire system including ASU and steam turbine (Stage 6)

Simulations using Aspen Plus®

MODEL VALIDATION



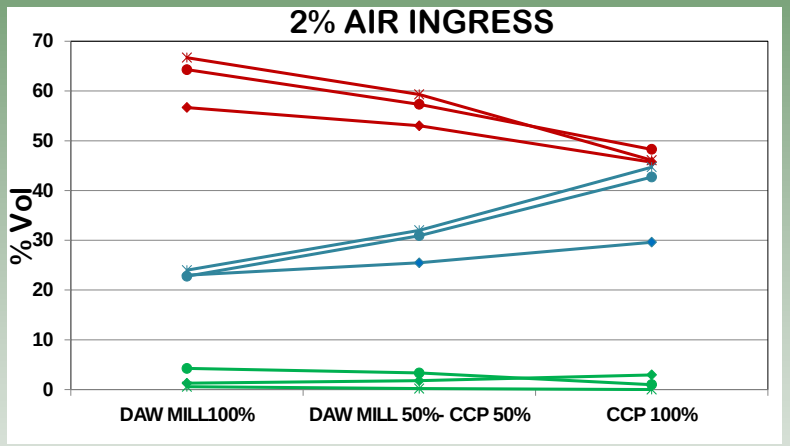
Box- plot of the Rate-based Model (Stage 3)

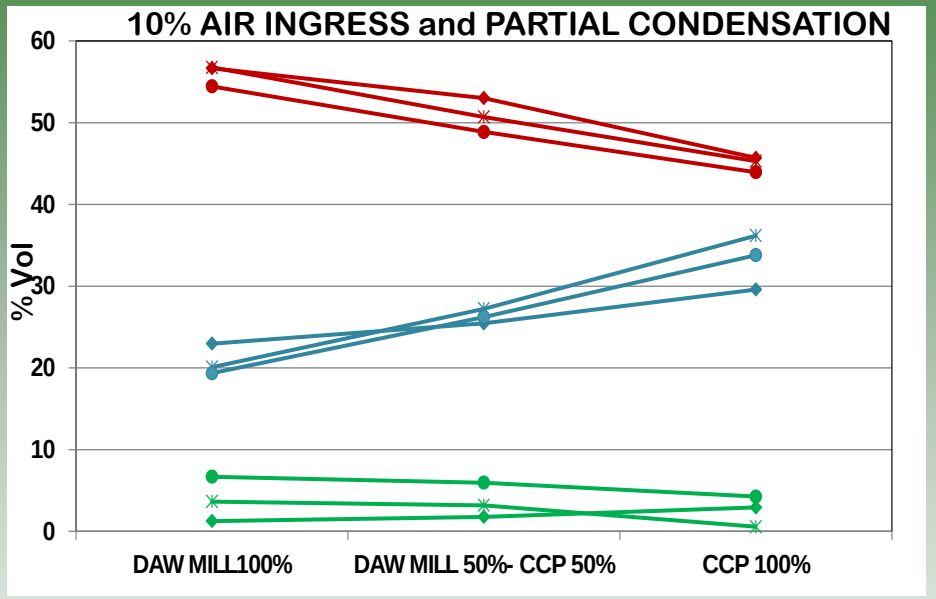


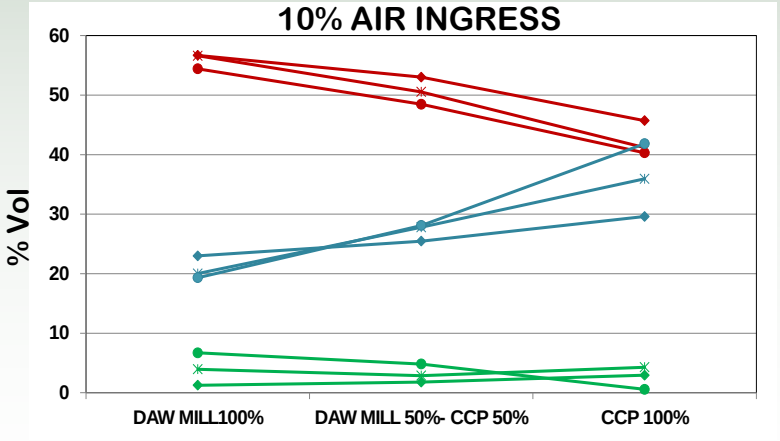
Interface of the rate-based model with partial condensation on the RFG in Aspen Plus (Stage 3)

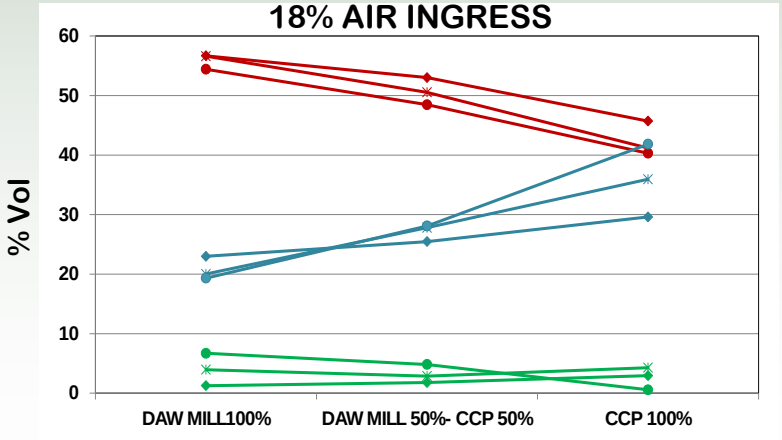
Simulations using Aspen Plus®

AIR INGRESS COMPARISON









Pilot plant: on-going modifications

WATER AND ACID SPECIES REMOVAL

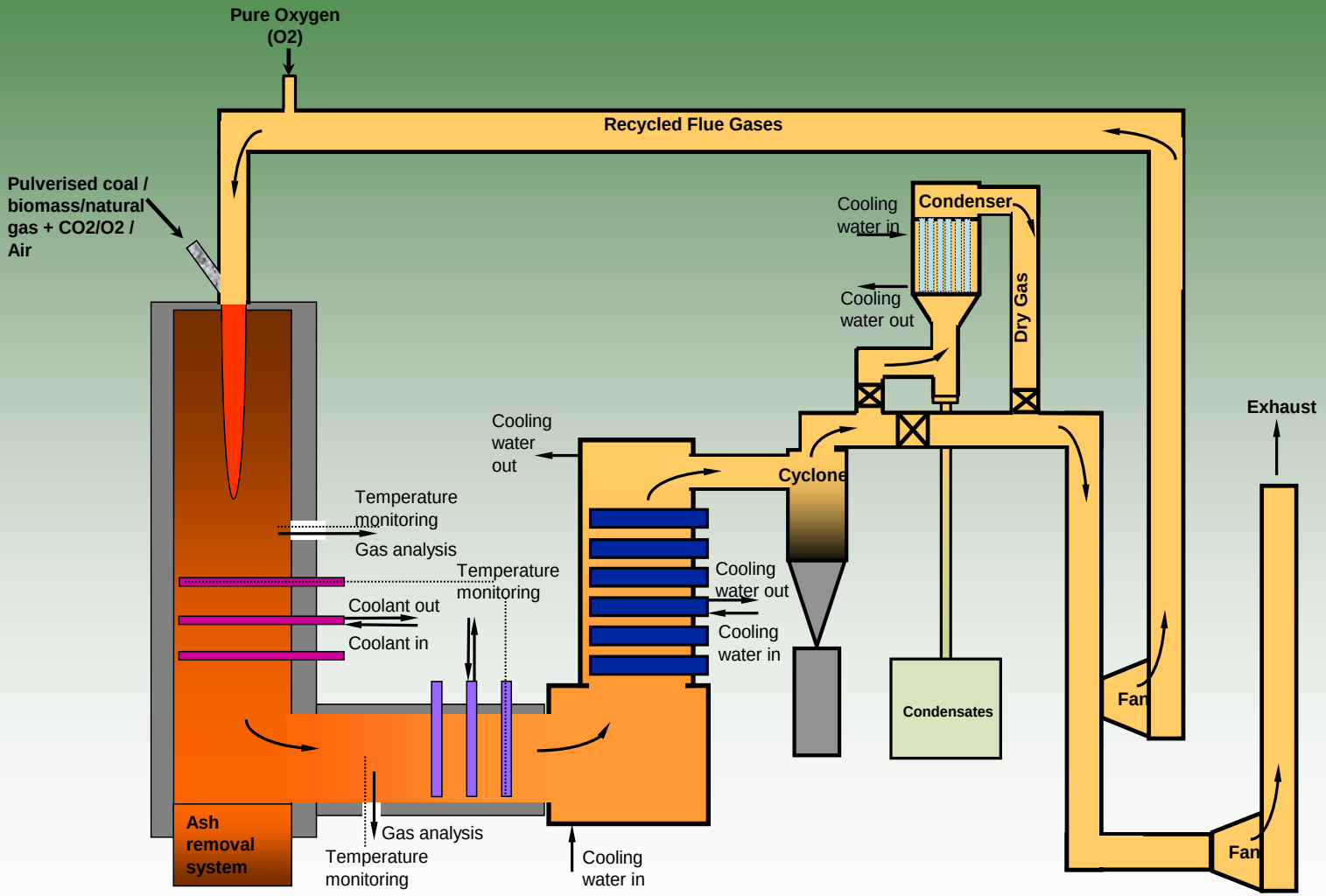
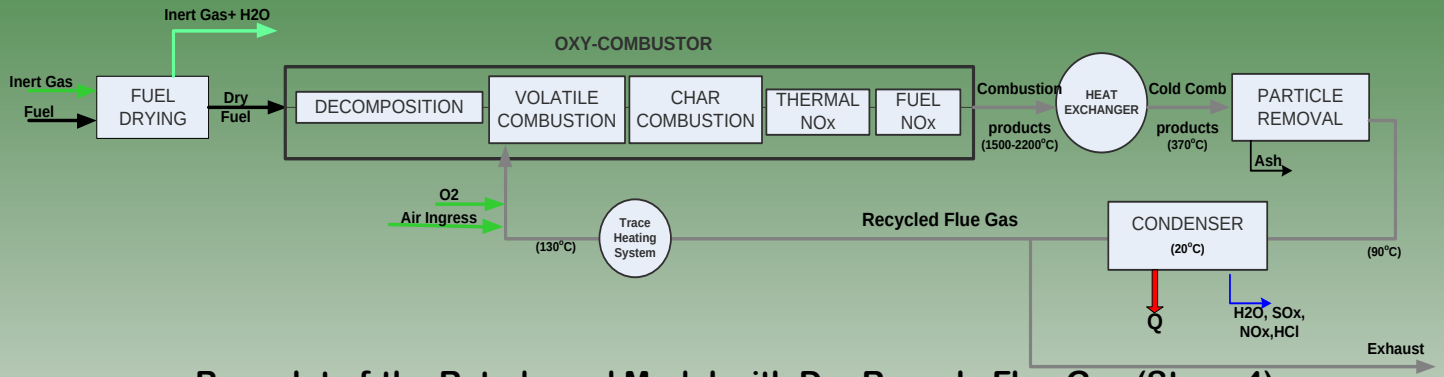


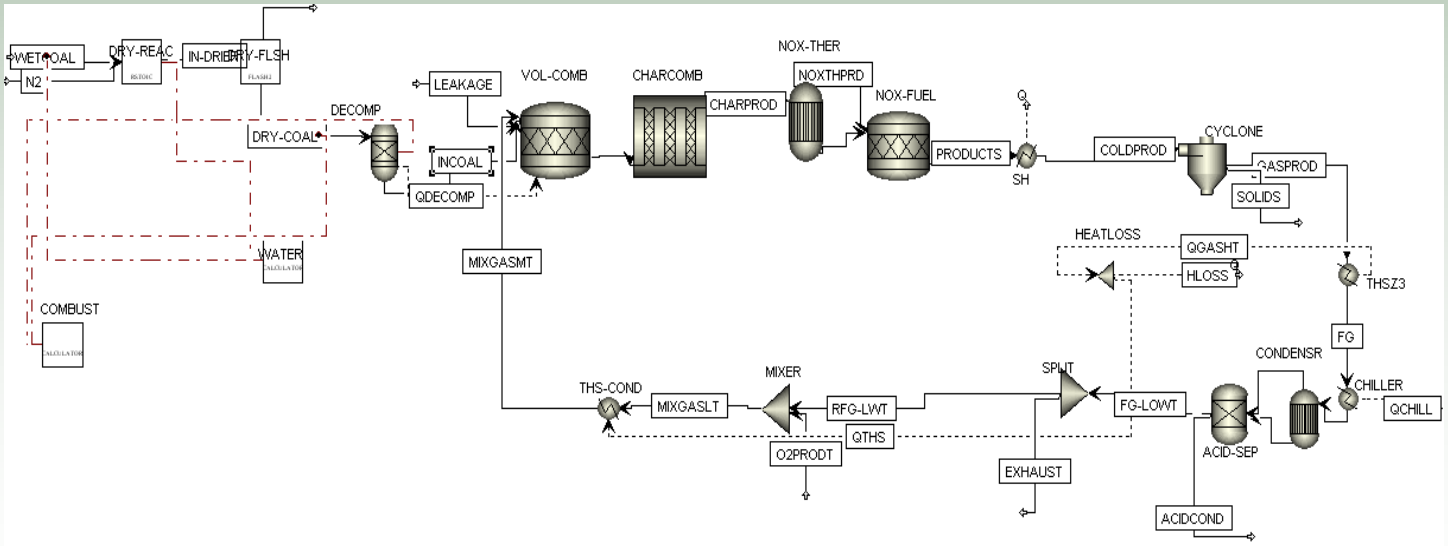
Diagram of 100kWth Oxy-Combustor with Condenser

Simulations using Aspen Plus®

DRY RECYCLE FLUE GAS



Box- plot of the Rate-based Model with Dry Recycle Flue Gas (Stage 4)

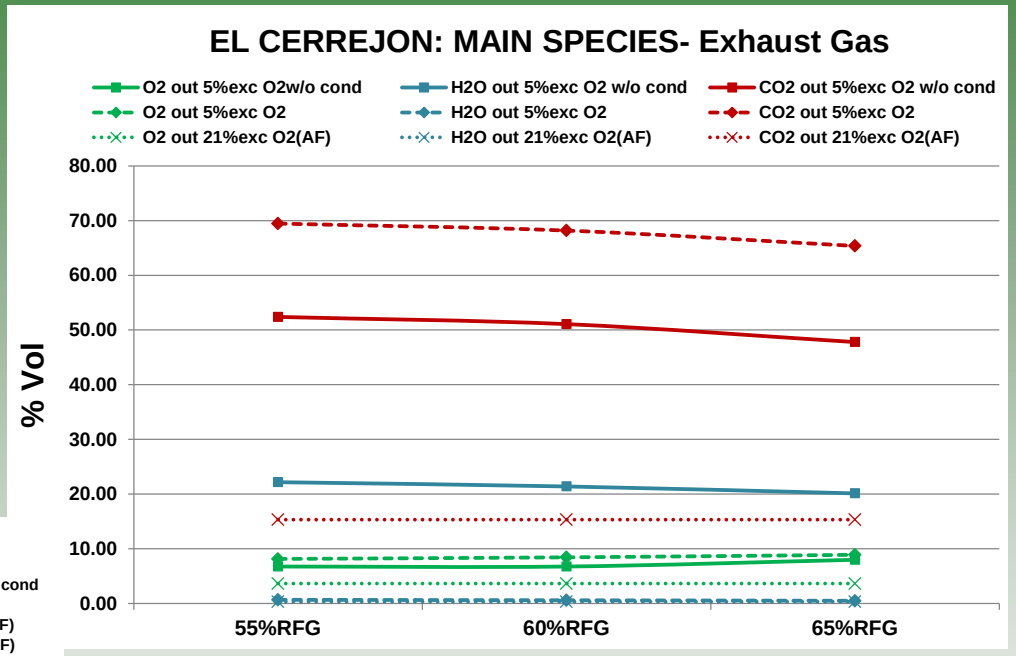


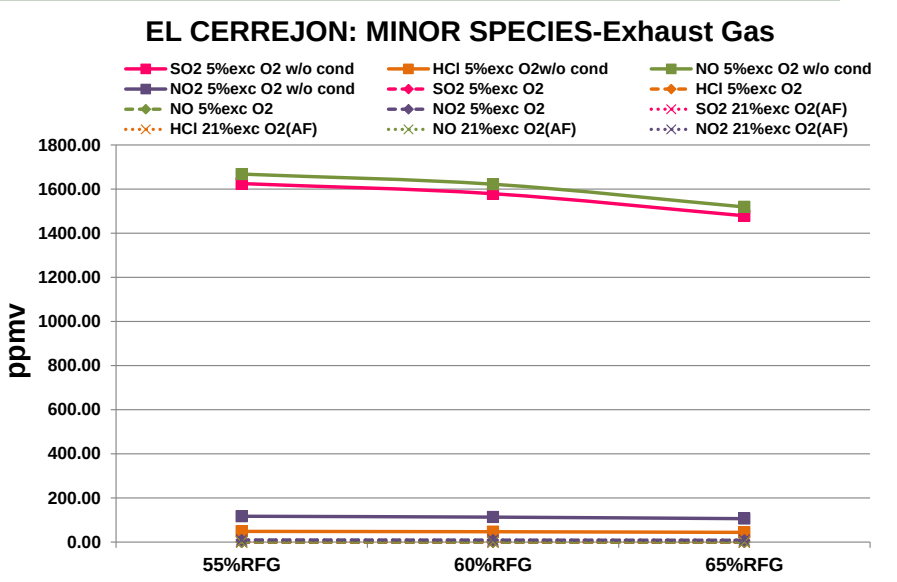
Interface of the rate-based model with dry RFG in Aspen Plus (Stage 4)

DRY RECYCLE FLUE GAS

EFFECT ON THE EXHAUST USING EL CERREJON COAL

- CO_2 increases 20% (v/v) as consequence of implementation of the condenser
- H_2O decreases at the same proportion to the increase of CO_2
- All minor species drop to near zero content in the exhaust gas, in the cases where the condenser was used



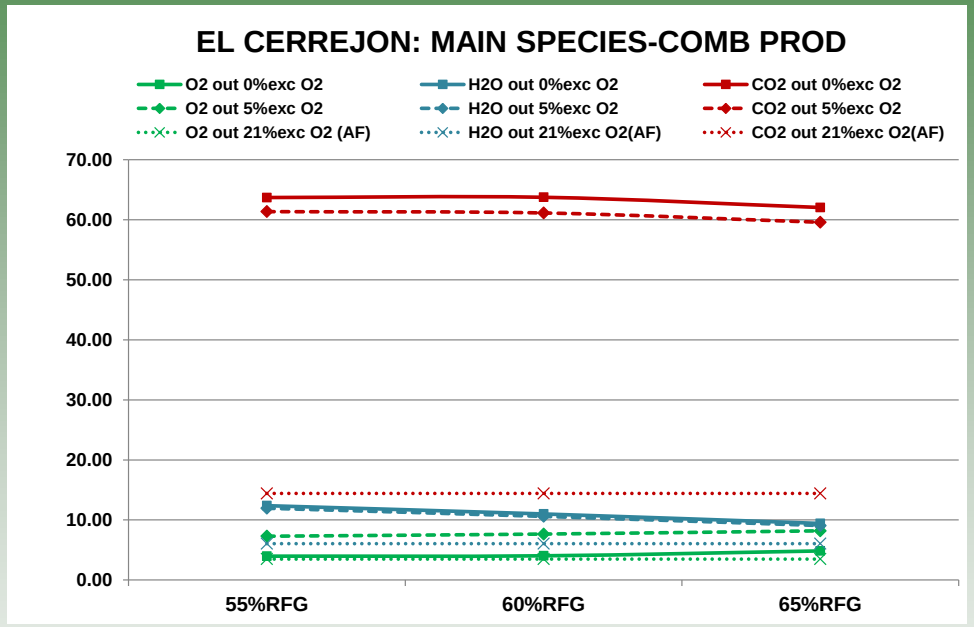


- Condensates composition:

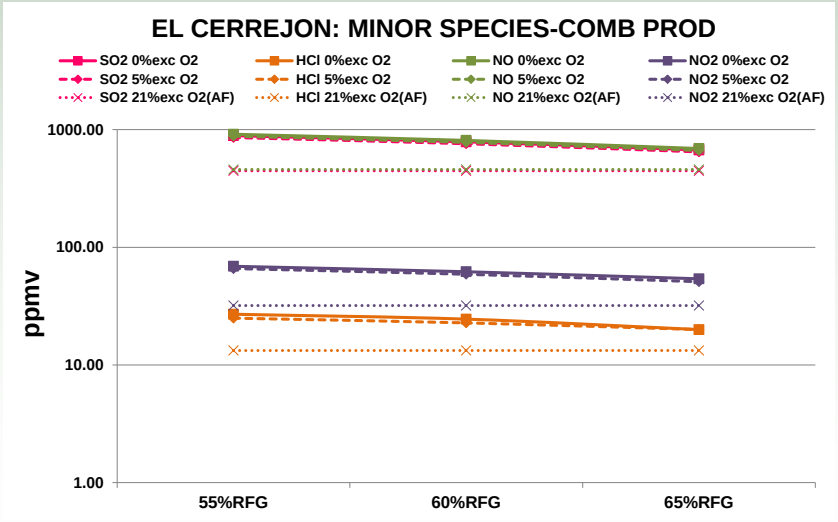
	H_2O (% v/v)	H_2SO_4 (% v/v)	HNO_3 (% v/v)	HCl (% v/v)
OXY-FIRING 60% RFG 5% O_2 exc	98	0.75	0.82	0.02
AIR-FIRING	98.37	0.77	0.84	0.02

DRY RECYCLE FLUE GAS

EFFECT ON THE COMBUSTION PRODUCTS USING EL CERREJON COAL



- Max. CO_2 at the exit of oxy-combustor 64%(v/v) versus 14.4 % (v/v) reached for air-firing
- No significant changes in H_2O content at different % RFG, between 9 and 12% (v/v)



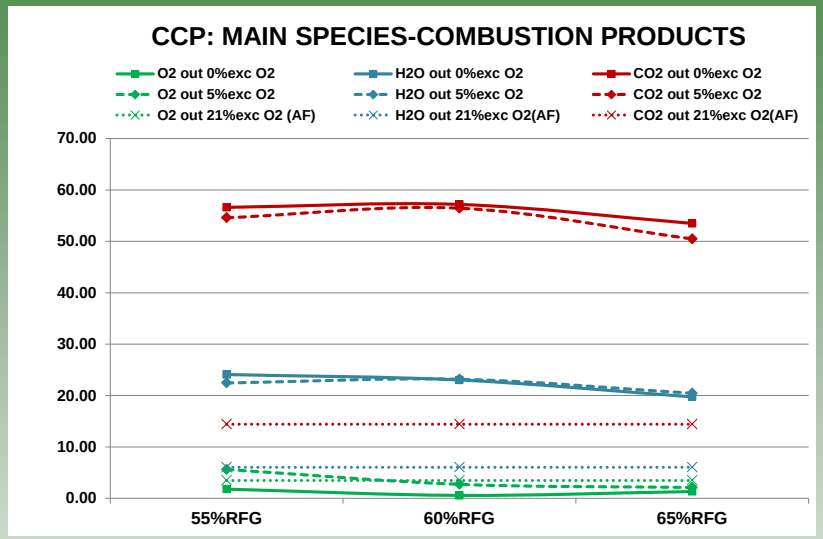
- Comparison with air-firing:
  - ✓ SO_2 : 760 vs 450 ppmv
  - ✓ HCl: 23 vs 13 ppmv
  - ✓ NO: 810 vs 460 ppmv
  - ✓ NO_2 : 59 vs 32 ppmv

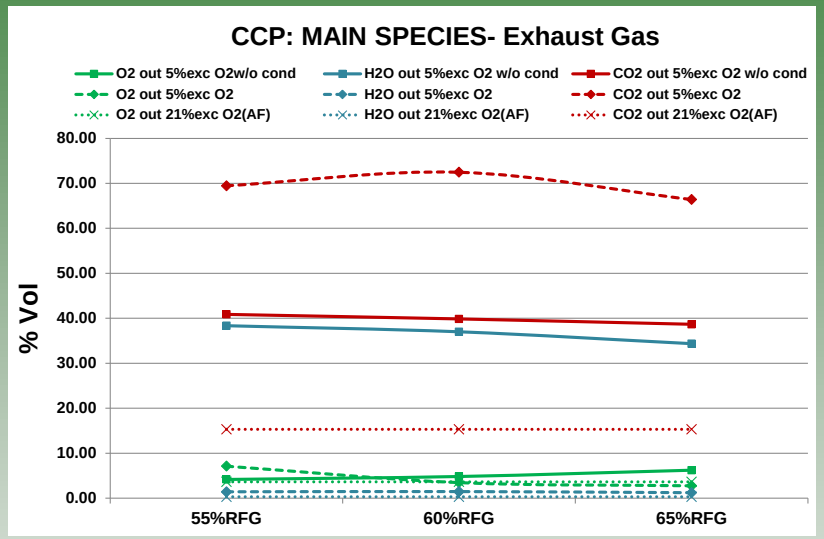
In general, oxy-firing almost doubles minor species concentration versus air-firing cases

- Minimal effect on the minor species when changing the % RFG and the excess of O_2 fed

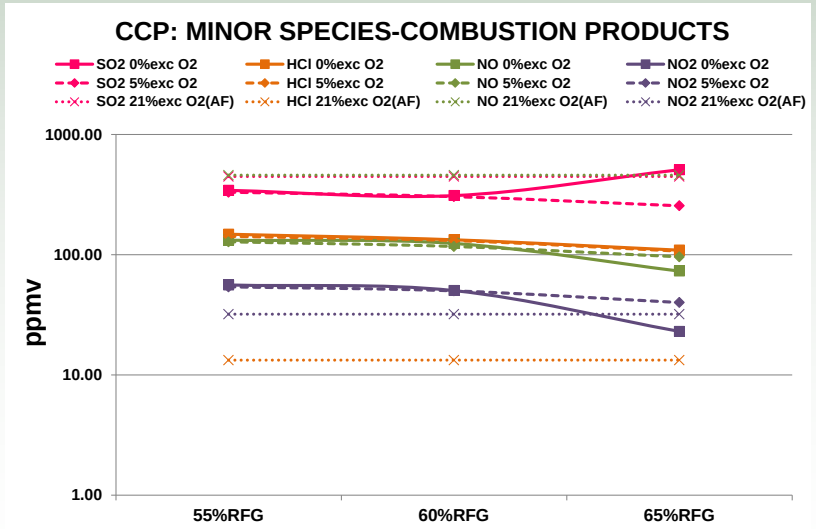
DRY RECYCLE FLUE GAS

EFFECTS USING CEREAL CO-PRODUCT





- Although the max CO_2 in the comb prod is lower for CCP than for 100% coal case, in the exhaust gas this concentration is higher due to the water vapour removal
- CO_2 increases 30% (v/v) as consequence of implementation of the condenser
- The effect of increasing the %RFG is shown by the dilution of the minor species. Exception: cumulative effect on SO_2 concentration

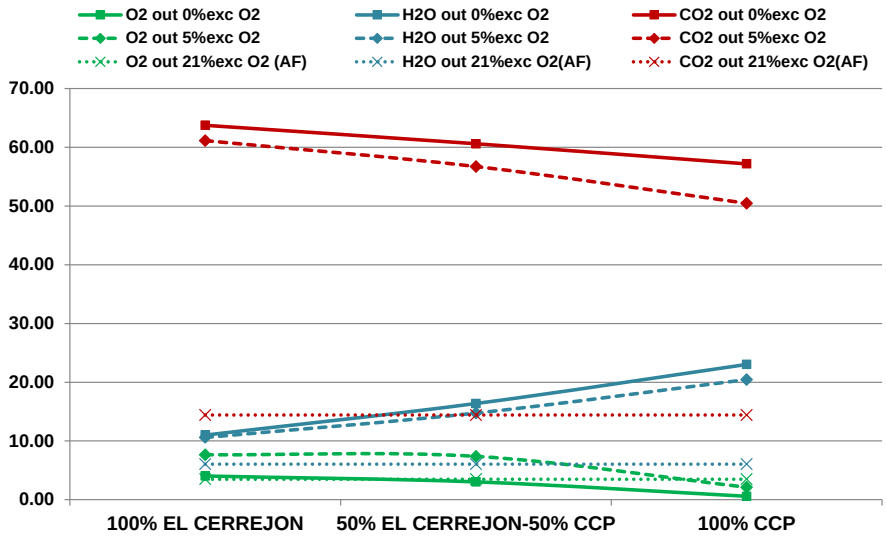


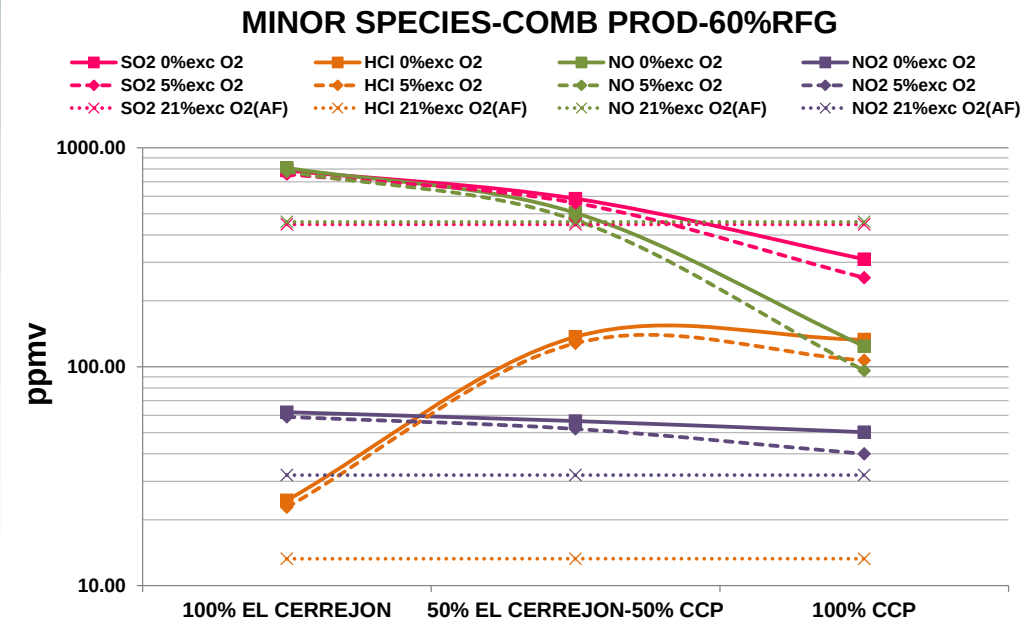
DRY RECYCLE FLUE GAS

FUELS COMPARISON

- Max. CO_2 decreases in the combustion products with higher content of biomass oxy-fired

- H_2O content when burning CCP increases:
  - ✓ By 10% comparing to oxy-firing 100%coal
  - ✓ By 14%comparing to air-firing case





- Marked decrease for SO_2 and NO contents when increasing the percentage of biomass

- Increase in the HCl content as result of the higher content of Cl in the elemental analysis of the biomass (0.17% (w/w) in CCP vs 0.02 % (w/w) El Cerrejon)

- No significant variation for NO_2 contents

SUMMARY

- Kinetic Simulation Model has been developed with acceptable agreement with experimental results
- Model validation has been carried out and helped to deduce the amount of air ingress into the process (10% of the total flue gas fed to the combustor)
- Simulation model including equipment for CO_2 purification predicts remarkable increase of the $\%CO_2$ contents
- Last stage under development :kinetic model including dry RFG,ASU, and steam turbine

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