THERMO CHEMICAL SIMULATION OF A COAL GASIFICATION PROCESS

(APPLYING WASTE CAPTURED CO_2 EITHER FROM COMBUSTION OR GASIFICATION)

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African Carbon Energy

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GTT-TECHNOLOGIES

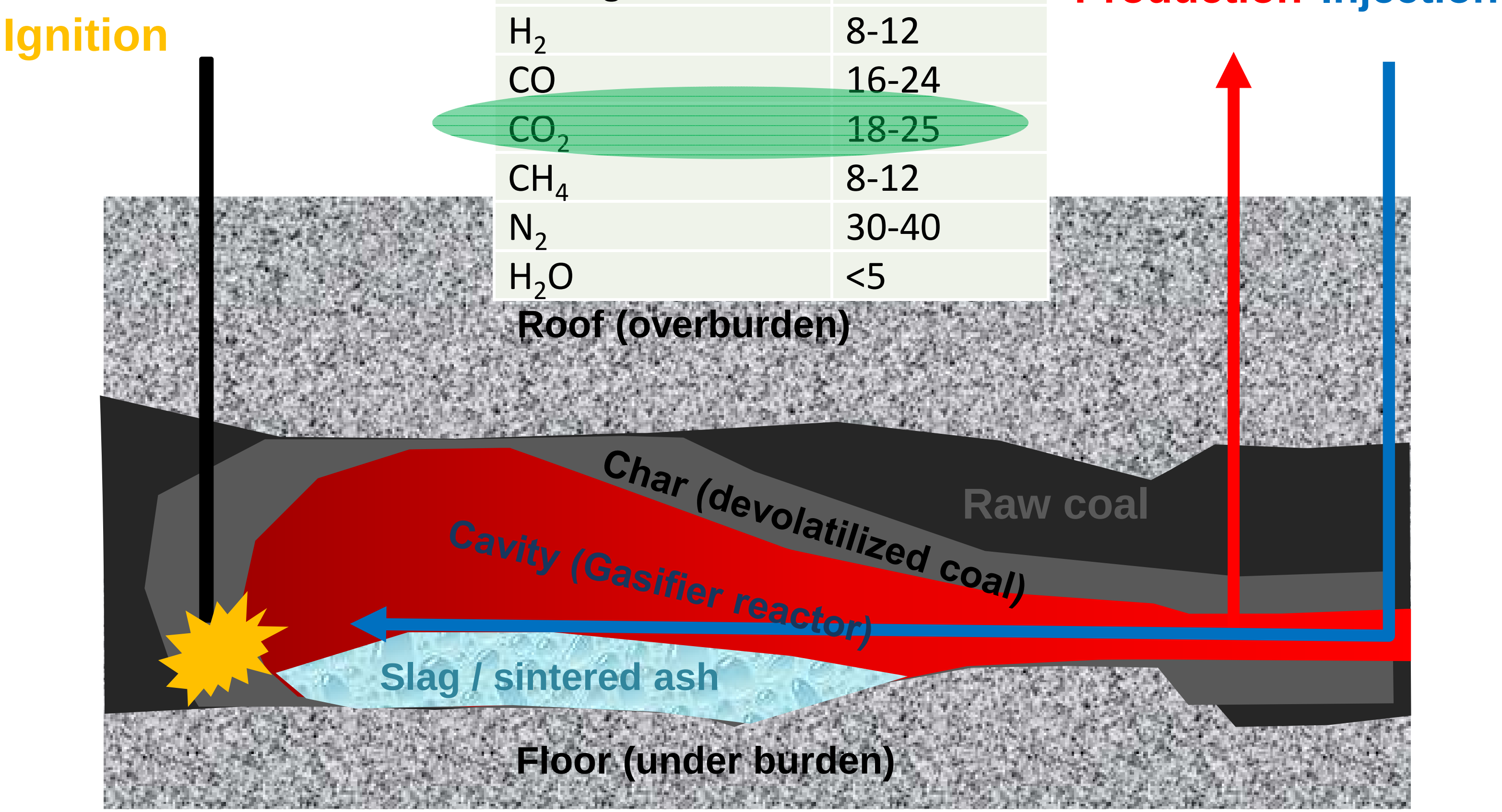
ROADMAP FOR THE PRESENTATION

- UNDERGROUND COAL GASIFICATION – EFFICIENT IN-SITU CO_2 CAPTURE AND CONVERSION

- Entrained flow Gasification
  E- Gas^{TM} (Reliance Industries) – AC Collins

UCG (OPERATION AND GAS COMPOSITION)

Average Raw Gas	Mol %
H_2	8-12
CO	16-24
CO_2	18-25
CH_4	8-12
N_2	30-40
H_2O	<5



COMBUSTION → GASIFICATION → PYROLYSIS → DRYING

COMBUSTION:

$C + ½ O_2 \rightarrow CO$

$C + O_2 \rightarrow$

$H_2 + O_2 \rightarrow H_2O$

GASIFICATION:

$C + CO_2 \rightarrow 2 CO$

$C + H_2O \rightarrow CO + H_2$

PURPOSE OF THIS STUDY

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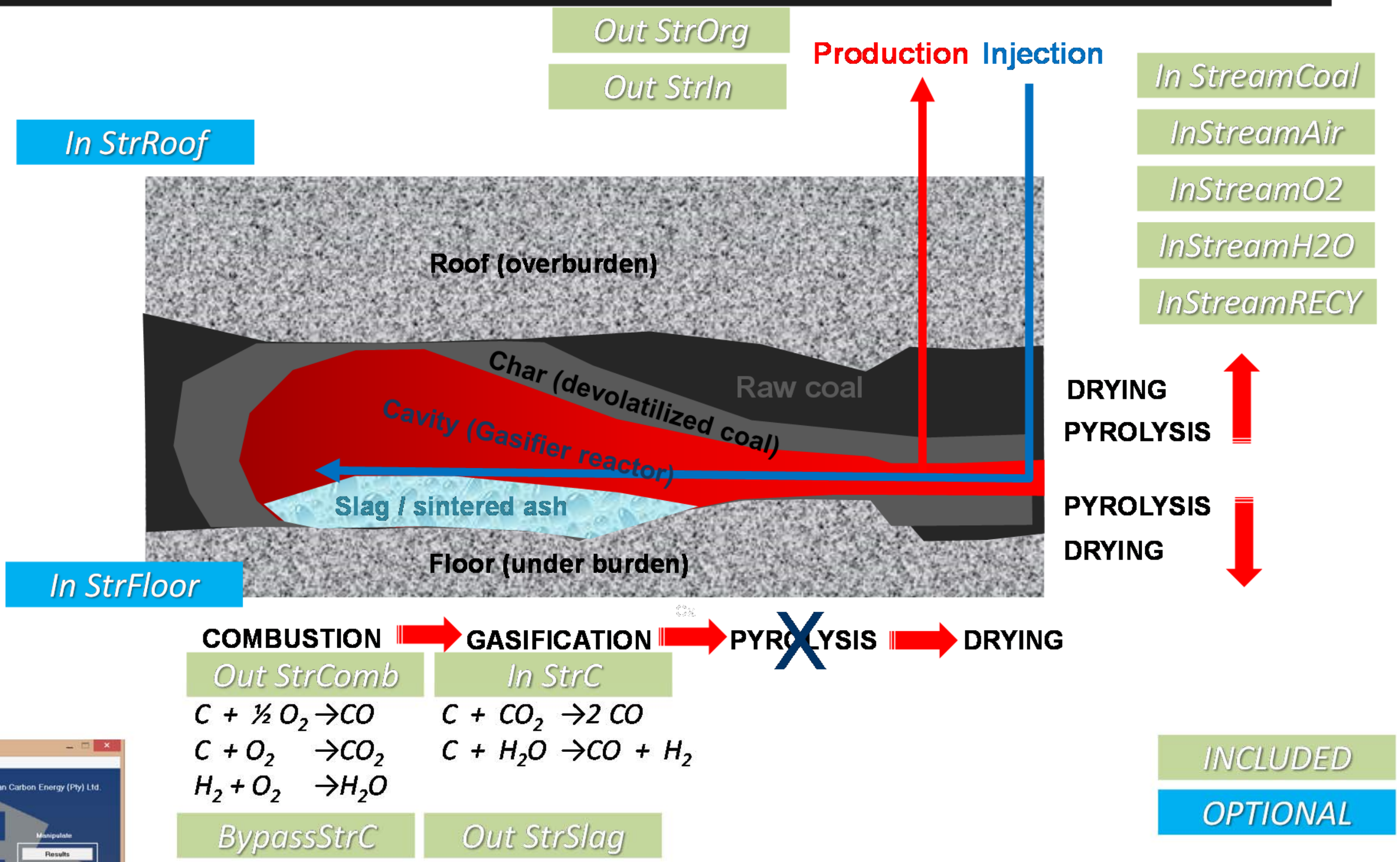
1. CO_2, **as gasification agent for UCG,** has received little attention and only studied by a few researchers to date - will be investigated on a thermo-equilibrium basis in this study.

2. Eftekhari, et. al., (2012) and others concluded further that Carbon Capture and Storage (CCS) in a geological form as sequestration within UCG is not practical and cannot result to a near zero-emission process - and **capture (utilizing) of CO_2 coupled with UCG** has to be studied in novel manners and approaches.

3. Evaluate under thermo-equilibrium conditions the positive influence which **CO_2 utilization as UCG gasification agent in parallel gasifiers** will positively influence the carbon emissions reduction and environmental footprint, gas quality, as well as reduction of CO_2 per ton coal when recycled to a second or third UCG cavity.

FACTSAGE™ THERMO EQUILIBRIUM APPROACH (SYNGAS)



SIMULATION PROCESS (Coal and operational inputs)

PROXIMATE (AR)	Mass %
Moisture	4.3
Fixed carboon	45.7
Volatile matter	19.2
Ash	30.8
ULTIMATE (DAF)	
C	78.9
H	4.3
N	2.1
S	0.9
O	13.9
ASH OXIDES (%)	
SiO_2	52.8
Al_2O_3	27.2
Fe_2O_3	4.9
P_2O_5	0.1
TiO_2	1.3
CaO	6.4
MgO	1.0
K_2O	0.5
Na_2O	0.4
SO_3	4.9
Trace Elements	0.5

Not included →

Property	Mass %
H_2O	2.9
H_2	0.15
CH_4	4.01
CO	0.98
CO_2	7.2
N_2	2.1
Tar and oils	5.6

- In situ coal = 50 000kg/hr
- Total agent (O_2 + Air) = 45 000kg/hr
- $C + O_2 \rightarrow CO_2$ (*Combustion zone*) – all O_2 molecules converted and remaining carbon to *Gasification zone*
- Water is the sum of all ground water and recycled water and will be kept at a constant for both G1 and G2.
- No contribution from roof and floor in this study – only individual coal seam
- 18 trace elements included

SIMULATION PROCESS (Gasifier 1)

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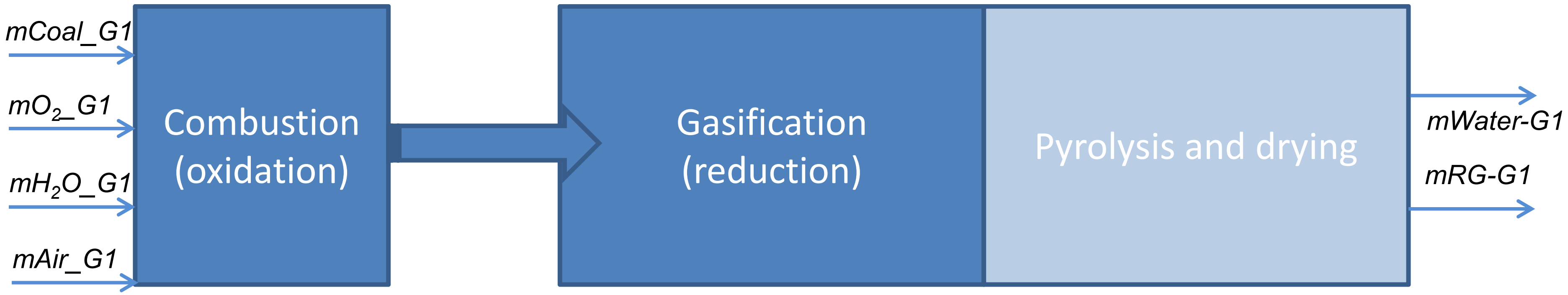


$C + ½ O_2 \rightarrow CO$

$C + O_2 \rightarrow CO_2$

$H_2 + O_2 \rightarrow H_2O$

$C + CO_2 \rightarrow 2 CO$

$C + H_2O \rightarrow CO + H_2$

Water-gas shift:

$CO + H_2O \rightarrow CO_2 + H_2$

Methane formation:

$C + 2 H_2 \rightarrow CH_4$

$CO + 3H_2 \rightarrow CH_4 + H_2O$

$3C + 2H_2O \rightarrow CH_4 + 2 CO$

SIMULATION PROCESS (Gasifier 2)

$C + ½ O_2 \rightarrow CO$

$C + O_2 \rightarrow CO_2$

$H_2 + O_2 \rightarrow H_2O$

$C + CO_2 \rightarrow 2 CO$

$C + H_2O \rightarrow CO + H_2$

<u>Water-gas shift</u>:

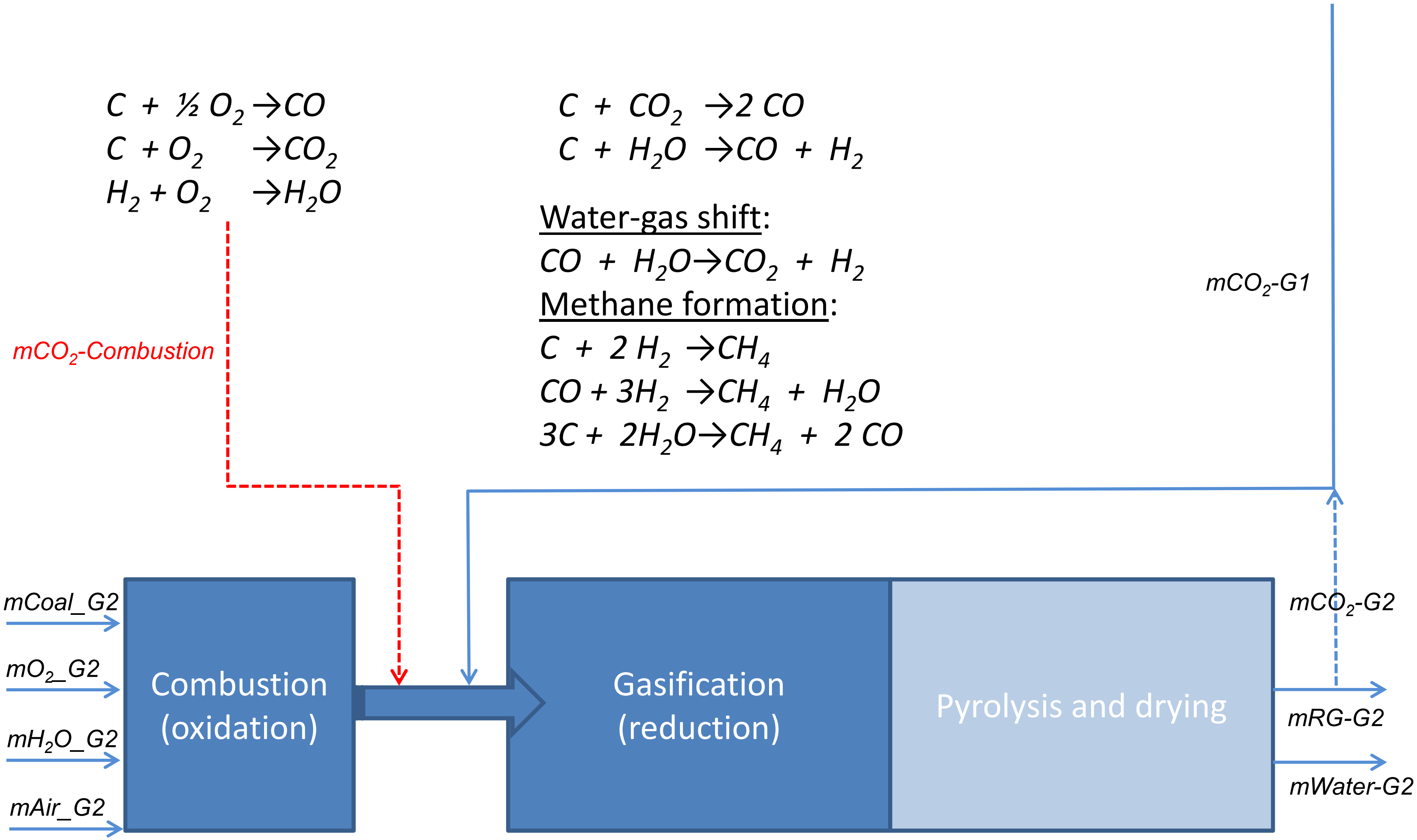
$CO + H_2O \rightarrow CO_2 + H_2$

<u>Methane formation</u>:

$C + 2 H_2 \rightarrow CH_4$

$CO + 3H_2 \rightarrow CH_4 + H_2O$

$3C + 2H_2O \rightarrow CH_4 + 2 CO$



SIMULATION PROCESS (G1+G2)

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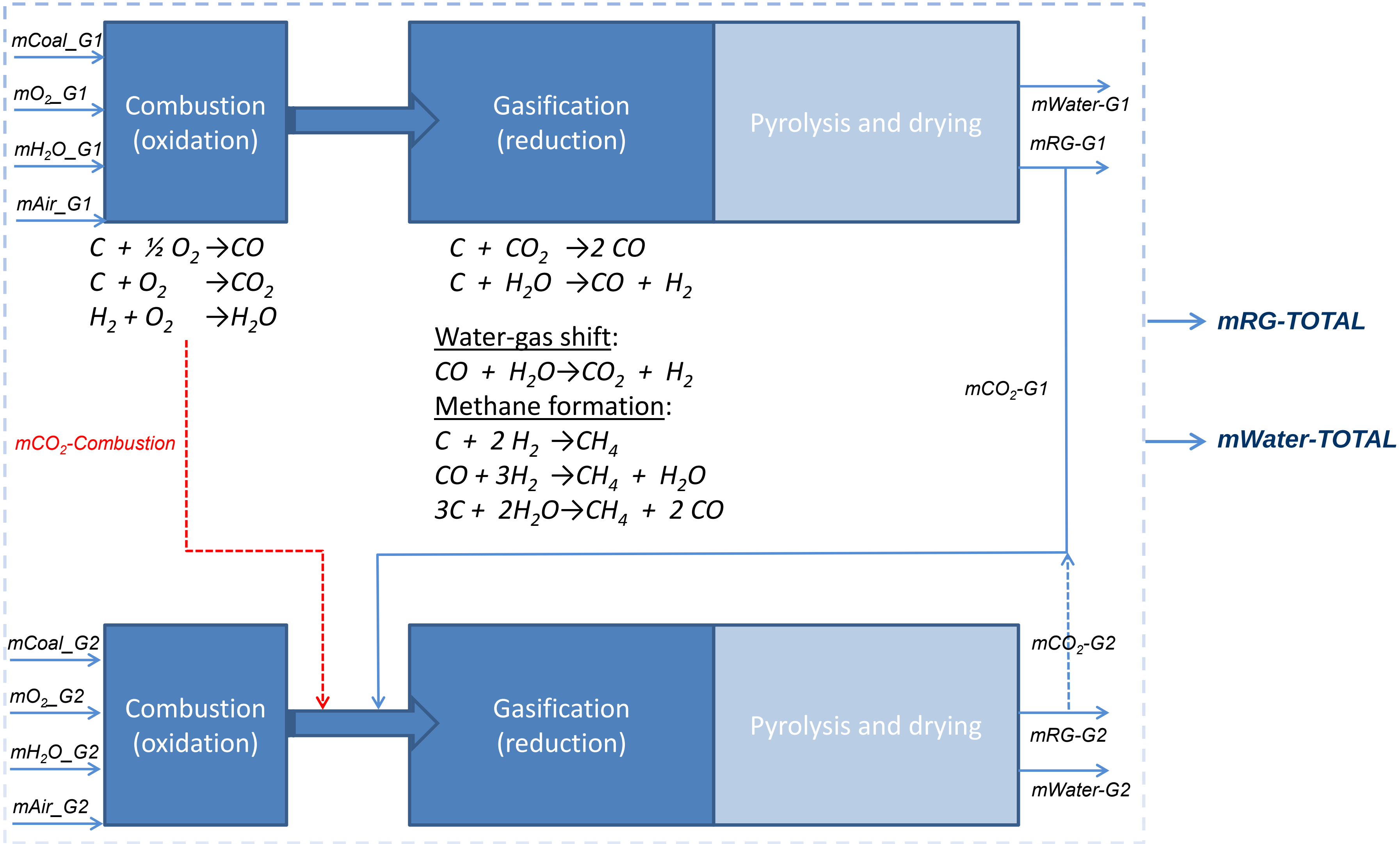
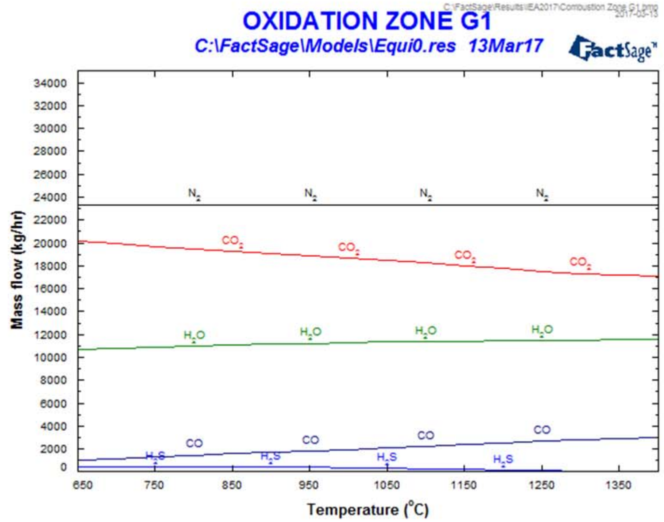
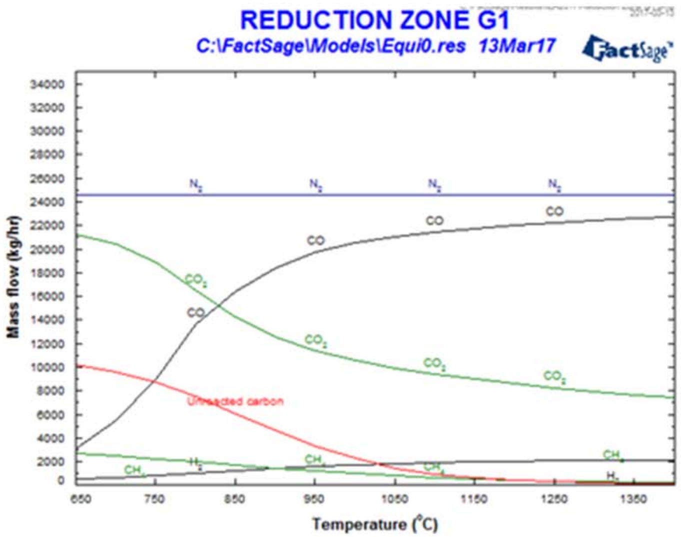


RESULTS (GASIFIER 1)



	kg/hr	mol %
CO	2 070	3.5
CO_2	17 563	18.9
N_2	24 080	40.3
H_2O	11 909	31.3
H_2S+COS	576	0.8
Reacted COAL	±15 000	

$C + O_2 \rightarrow CO_2$ (*Combustion zone*) – all O_2 molecules converted and remaining carbon to *Gasification zone*



	kg/hr	mol %
H_2	341	7.2
CO	20 153	30.6
CO_2 (mCO_2_G1)	**10 556**	**10.2**
CH_4	3 394	9.0
N_2	25 975	39.5
H_2O	1 144	2.7
H_2S	577	0.7
Raw gas (mRG_G1)	62 140	
Unconverted Coal	101	

RESULTS (GASIFIER 2)

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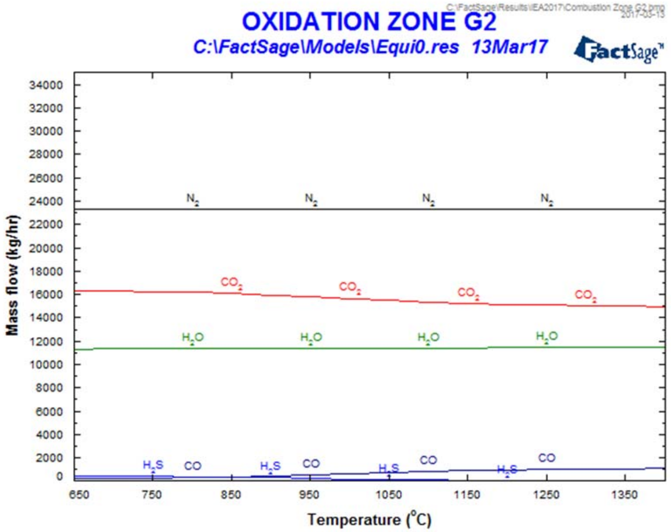
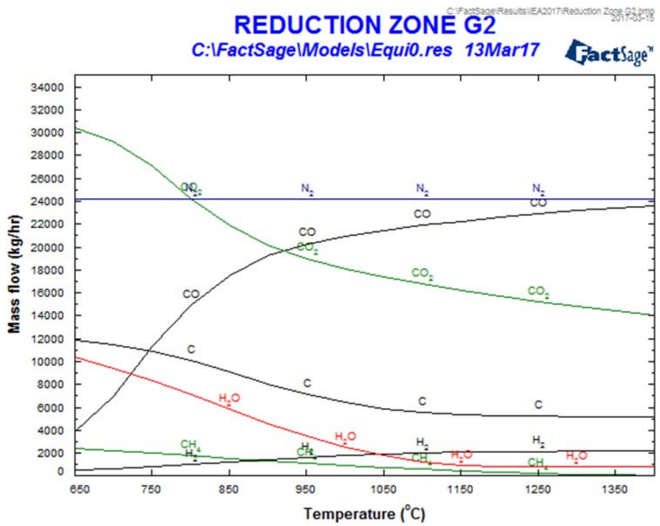


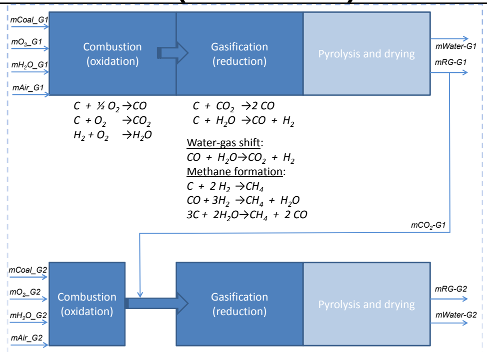
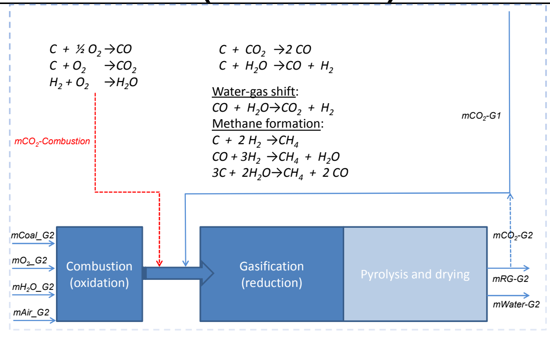
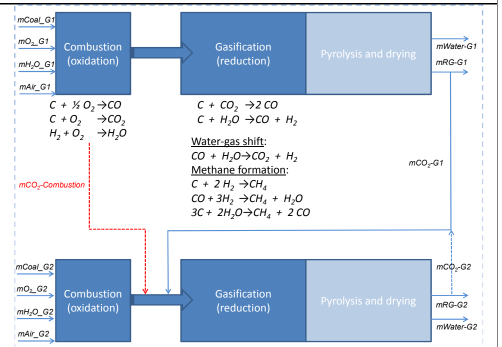


1. *mCO_2_G1 = 10 556 kg/hr*
2. *mAir_G2 = mAir_G1 - mCO_2_G1*

	kg/hr	mol %
CO	799	1.5
CO_2	15 493	18.6
N_2	23 727	44.7
H_2O	11 795	34.3
H_2S+COS	454	0.7
Reacted COAL	17 280	

	kg/hr	mol %
H_2	356	7.3
CO	22 238	32.8
CO_2 (mCO_2_G2)	13 590	12.8
CH_4	3 537	9.1
N_2	23 485	34.6
H_2O	1 192	2.7
H_2S	601	0.7
Raw gas (mRG_G2)	64 999	
Unreacted COAL	5000	

RESULTS (COMBINED G1 + G2)

INDEX	G1 (BASE CASE)	G2 (CO2 RECYLE)	COMBINED G1+G2
Flow scheme			
Coal usage (kg/hr)*	49 800		
CO_2 produce (kg/hr)	10 556 (recyle)		
Oxygen (kg/hr)**	14 512		
Syngas (kg/hr)***	62 140		
CO_2:Syngas	0.17		
CO_2:Coal	0.21		
Nitrogen (kg/hr)	25 975		

* Total coal for equilibrium
** Total oxygen molecules air + pure oxygen
*** Syngas including CO_2
**** Excluding CO_2 from G1 recycled

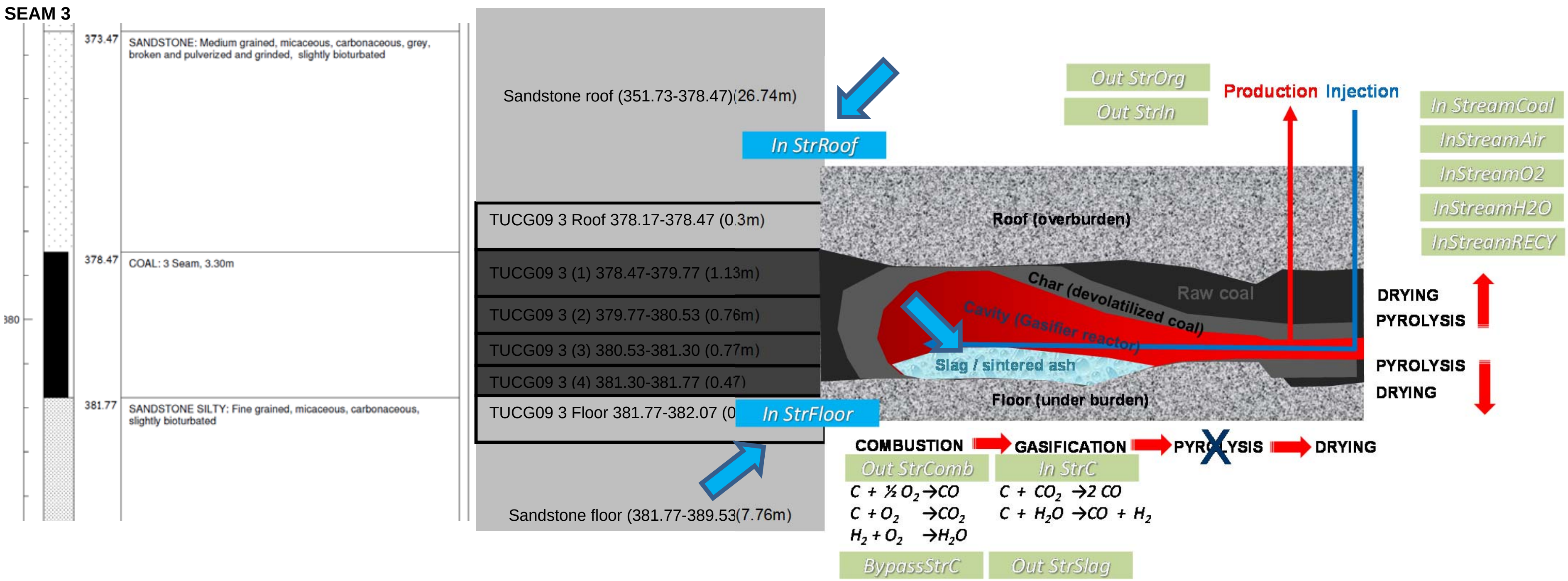
CONCLUSIONS

- Thermo-equilibrium add value in
  - determining the optimized process conditions for a specific feed and operating scenario
  - coal ash fusibility characteristics & slag-profile behaviour prediction to prevent operational shut-downs
  - new flow schemes during the concept and design phase

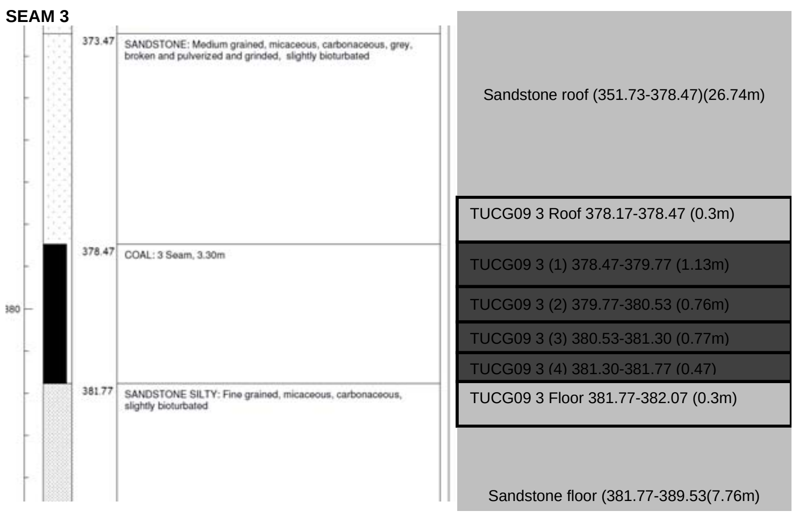
- Coal composition from either core drillings or actual mine samples can be used as input for the complex equilibrium calculations using FACTSAGE™.

NEXT STEPS IN PROGRESS

(Influence of roof, floor and slag on CO_2 capture and flow temperature with recycling)



NEXT STEPS IN PROGRESS



Sample naming	Anatase	Dolomite	Halite (Sodium Chloride)	Kaolinite	Micro-cline	Muscovite	Plagioclase	Pyrite	Quartz	Rutile	Siderite
	(TiO_2)	($CaMg(CO_3)_2$)	(NaCl)	($Al_2(Si_2O_5)(OH)_4$)	($KAlSi_3O_8$)	(KAl3Si3O10(OH)2)	((Na,Ca)(Si,Al)4O8)	(FeS2)	(SiO2)	(TiO2)	(FeCO3)
TUCG09/3 ROOF/1	0.7	0.7	0.61	17.48	12.47	5.20	16.12	0.47	45.17	1.12	0.00
TUCG09/3 /1 TUCG09/3 /2 TUCG09/3 /3 TUCG09/3 /4	4.3	0.0	0.00	52.50	5.96	5.17	3.39	2.33	24.78	1.58	0.00
TUCG09/3 LOOR/1	1.3	0.9	0.07	37.74	9.08	8.75	1.96	0.39	38.60	1.14	0.11
TUCG09/1 /1	2.2	0.0	0.34	23.20	6.18	11.25	5.20	1.50	49.24	0.93	0.00

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