Simulation and validation of CO_2 mass transfer processes in aqueous MEA solutions with Aspen Plus at CO_2 Technology Centre Mongstad

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Outline

- Introduction
  - CO_2 Technology Centre Mongstad

- Experimental
  - Amine plant absorber specifications
  - MEA campaigning (2013/2014 and 2015)
  - Aspen Plus modeling work at TCM

- Results and discussion
  - Overall simulation results
  - Temperature absorber profiles
  - CO_2 loading and enhancement factor absorber profiles
  - Driving forces and flux absorber profiles

- Concluding remarks

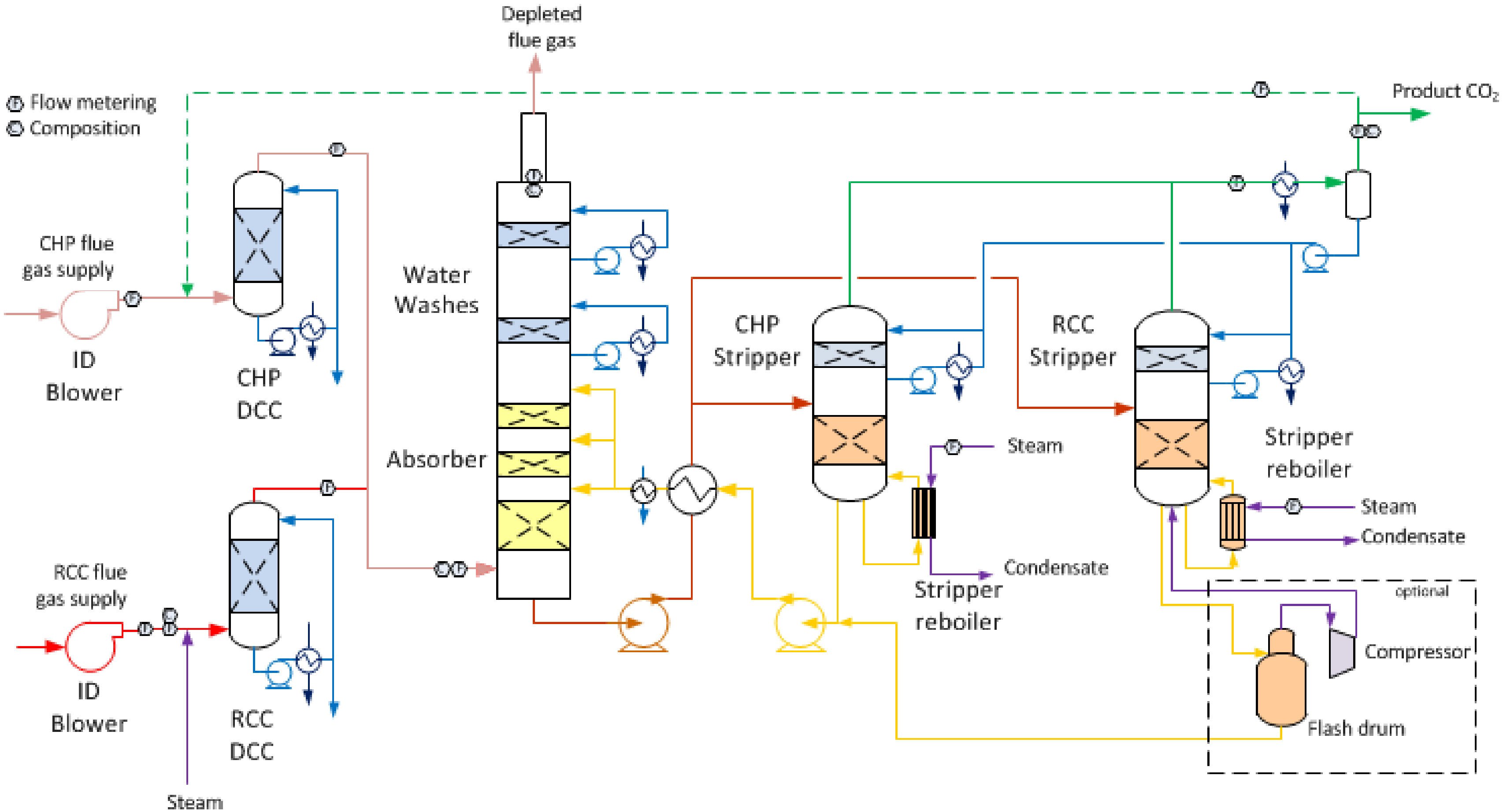
CO_2 Technology Centre Mongstad

- Located at the Mongstad industrial site
  - Oil refinery (flue gas with ~13% CO2)
  - Gas fired power plant (flue gas with ~3.5% CO2)

- Amine plant
  - Design & construction: Aker Solutions and Kværner
  - Campaigns: Aker Solution, Shell Cansolv
- Chilled ammonia plant
  - Design & construction: Alstom
  - Campaigns: Alstom

- TCM Owners: Gassnova (Norwegian state), Statoil, Shell, Sasol
- Purpose of TCM is to test, verify, and demonstrate CO_2 removal technologies
  - TCM does not develop CO_2 removal technologies

TCM Amine plant

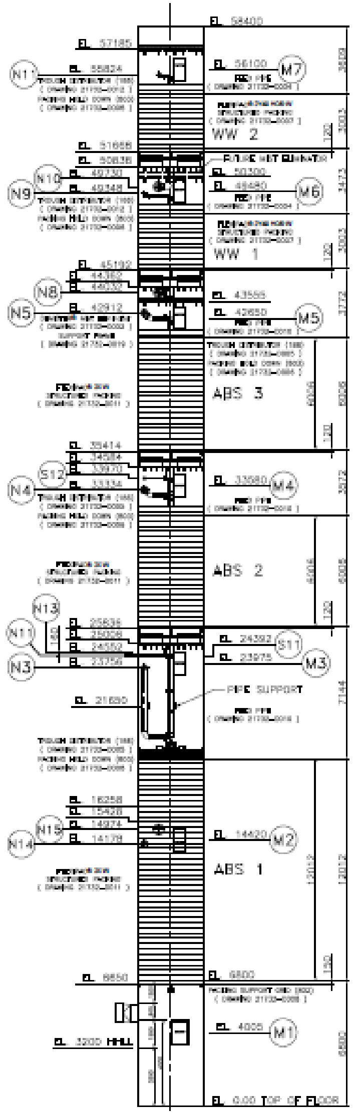


TCM Amine plant – absorber

- Absorber results are well suited for simulator verification (e.g. Aspen Plus)
- Verifies (and tunes) mass transfer/kinetic and equilibrium correlations

- Absorber structure
  - 62 meter total height
  - 3.55m x 2m = 7.1m^2 cross sectional area
  - Koch Glitsch structured stainless steel packing
    - 3m + 3m = 6m water wash section
    - 12m + 6m + 6m = 24m absorption section
  - Collector trays and redistributors
  - Space available for (future) intercooler connections
  - 3m absorber sump
  - Demisters upstream and downstream water wash sections

- Instrumentation & sampling ports
  - 4 temperature sensors in radial plane at ~1m elevations
  - Solvent sampling stations at solvent inlet, outlet, and between sections
  - Differential pressure sensors over each section
  - Gas and liquid flow meters at inlet and outlet flows



MEA campaigns at TCM

- TCM conducted MEA campaigns;
  - Dec 2013 – Feb 2014 (in collaboration with Aker Solutions)
  - July 2015 – present (gas phase instrumentation heavily upgraded, results not considered here)

- MEA concentrations ranging 30 – 40 wt% on CO_2 free basis
  - Varying concentration causes different absorber temperature and mass transfer profiles → ideal for simulator verifications

- Purpose of MEA campaigns;
  - Generate baseline results for comparison to commercial vendor technologies
  - Generate non-confidential results for easier and more straight-forward publishing, sharing, and knowledge build-up
  - Etc..

Aspen Plus modelling at TCM

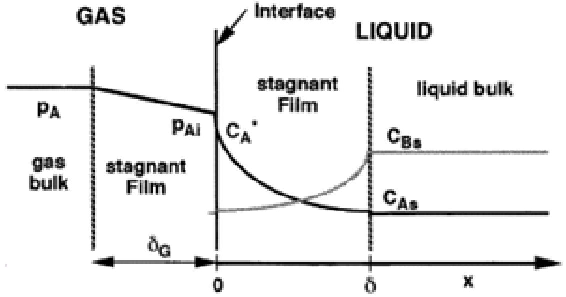
- TCM is using commercial available Aspen Plus simulator
  - Version 7.0, 7.1, 7.3, and now upgrading to 8.6
  - Developed Excel tool for easier user interface with Aspen Plus v7.x
  - Adjustments to the physical solubility of CO_2 and refitted thermodynamic interaction parameters in v7.3 (collaboration with NTNU)
    - No further internal simulator development

- Simulator flow sheet resembles plant as much as possible
  - Heat exchanger coupled absorber/stripper, water wash sections, 2 stripper, and vapor compressors system, etc. implemented
  - Bravo et al. mass transfer/liq hold-up correlation, Chilton & Colburn heat transfer correlation, RadFrac/eNRTL mass transfer/thermodynamic model, etc.
  - Simulation procedure:
    - Input: gas inlet temp & flow, liq. inlet flow & α_{CO2}, MEA conc., capture rate, and packing height.
    - Model tuning by interfacial area factor → here: 0.55

Absorber modelling and analysis

- Reactive gas-liquid mass transfer processes simplified;

$$A_{gas} + B_{liq} \rightleftharpoons C_{liq} + D_{liq}$$



- Assume;
  - Mass transfer resistance at both gas and liquid side.
  - Reactive mass transfer (kinetics) can be described by the enhancement factor *E*
  - Physical gas solubility described by partition coefficient *m* and assumption of equilibrium at interface *i*
- Well-known mass transfer relations;
  - Liquid side mass transfer; $J_A = k_L . E\left(\frac{c_A^{G,i}}{m} - c_A^{L,b}\right)$
  - Gas side mass transfer; $J_A = k_G . \left(c_A^{G,b} - c_A^{G,i}\right)$
  - Combining and rearranging yields; $E = \frac{J_A m}{\left(c_A^{b,G} - m c_A^{b,L} - \frac{J_A}{k_G}\right) k_L}$
- At each discretization stage, enhancement factor (E) and flux can be determined
  - Provides the rate of absorption into a reactive solvent to the rate into a non-reactive/physical solvent

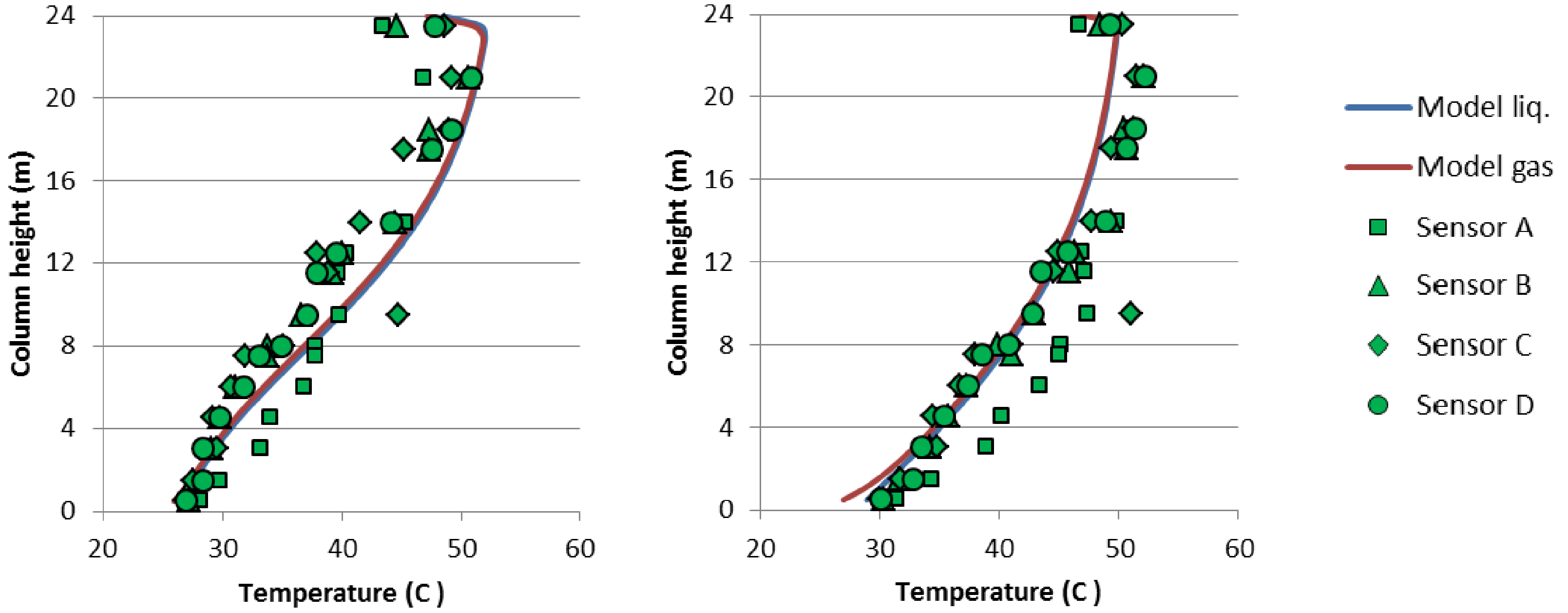
Absorber modeling results

- Overall absorber modeling input & results

Parameter	**Unit**	**30 wt% MEA**		**40 wt% MEA**	
		Plant	**Simulation**	**Plant**	**Simulation**
Flue gas flow rate	Sm^3/hr	46.600	46.600	59.000	59.000
Flue gas CO_2 conc. (CHP)	[vol%]	3.57	3.57	3.27	3.28
Depleted flue gas CO_2 conc.	[vol%]	0.43	0.42	0.34	0.27
Capture rate	[%]	88.5	88.5	89.9	91.9
Solvent flow rate	kg/hr	55.000	55.500	46.700	45.100
Lean solvent loading	[-]	0.25	0.25	0.19	0.21
Rich solvent loading	[-]	0.49	0.46	0.47	0.45
Packing height	m	24	24	24	24
Anti-foam injected		no	n/a	yes	n/a

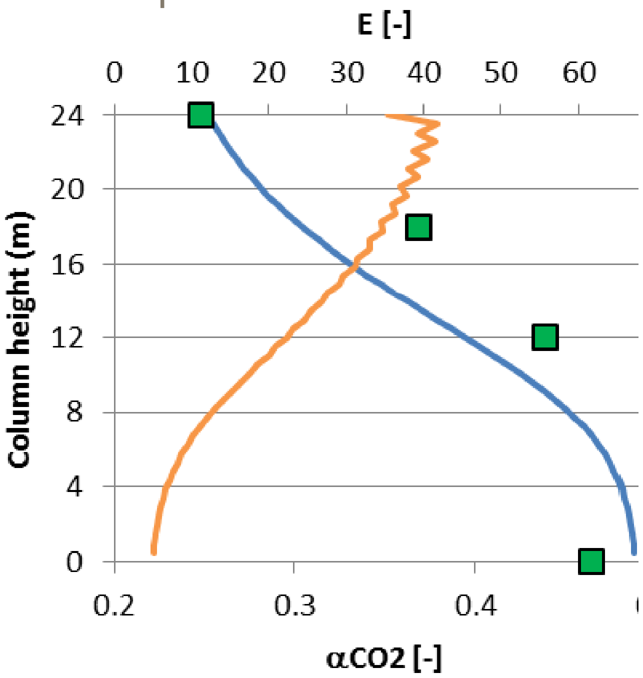
Results – temp profiles 30 and 40 wt%

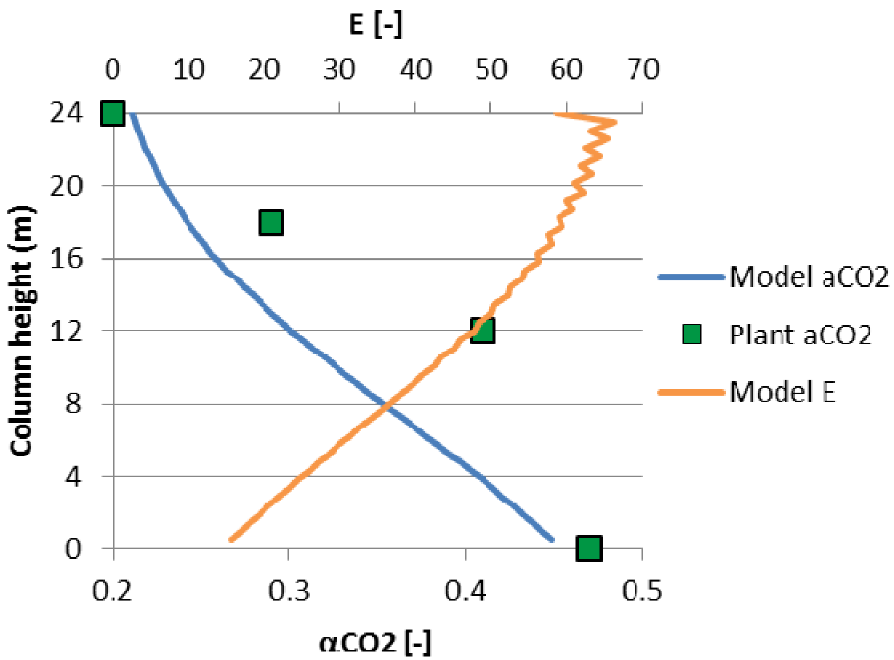
- Good temperature predictions
- 40 wt% → higher temp as more CO_2 absorbs → exothermic rxn.



Results – α_{CO2} and E profiles 30 and 40 wt%

- OK α_{CO2} prediction → mass transfer models may need further improvement
- Reactive chemical MEA absorbent provides highest “impact” on mass transfer at absorber top





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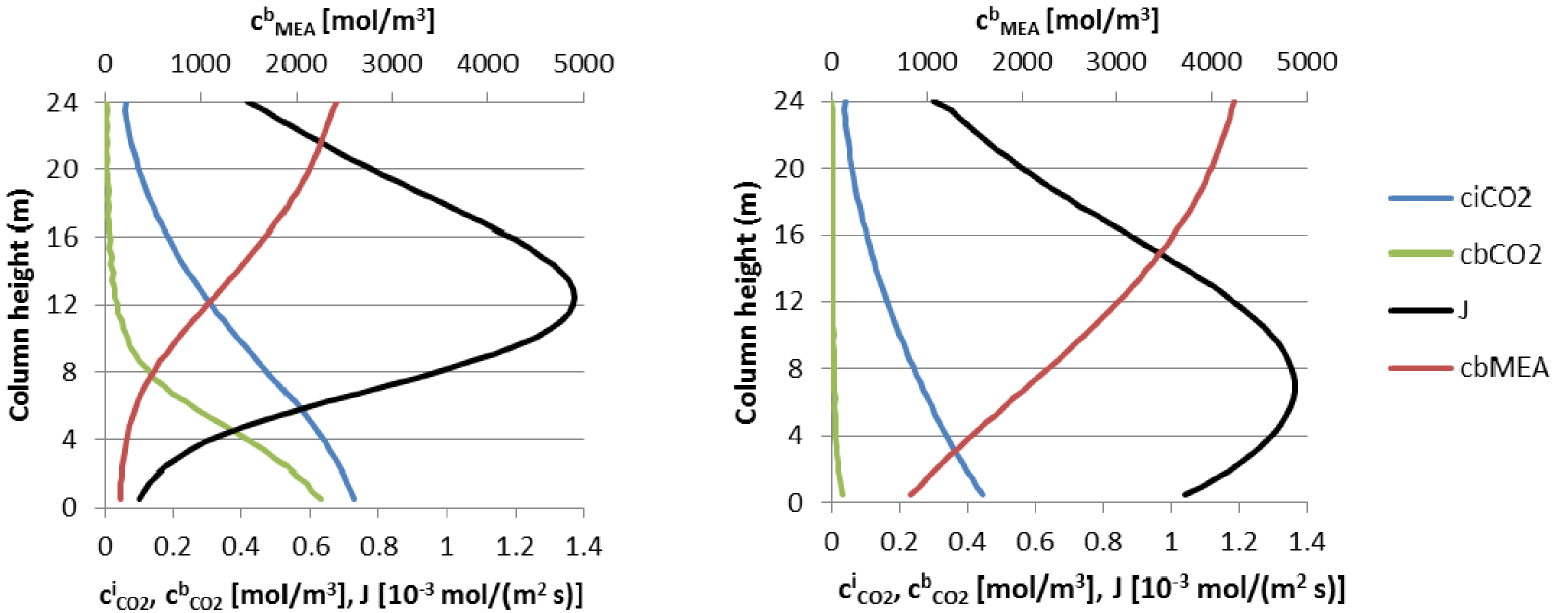
Results – driv. forc., flux profiles 30 and 40 wt%

- Good driving forces throughout, highest flux and driving forces in middle of absorber
  - Top approaching equilibrium due to very low CO_2 gas content → importance of good gas phase instrumentation at absorber to avoid top pinching
  - Bottom approaching equilibrium due to increased P_{CO2} VLE due to increase α_{CO2}
- Simulated (!) driving force pattern 40 wt% differs → should look similar from exp. α_{CO2} profile



Concluding remarks

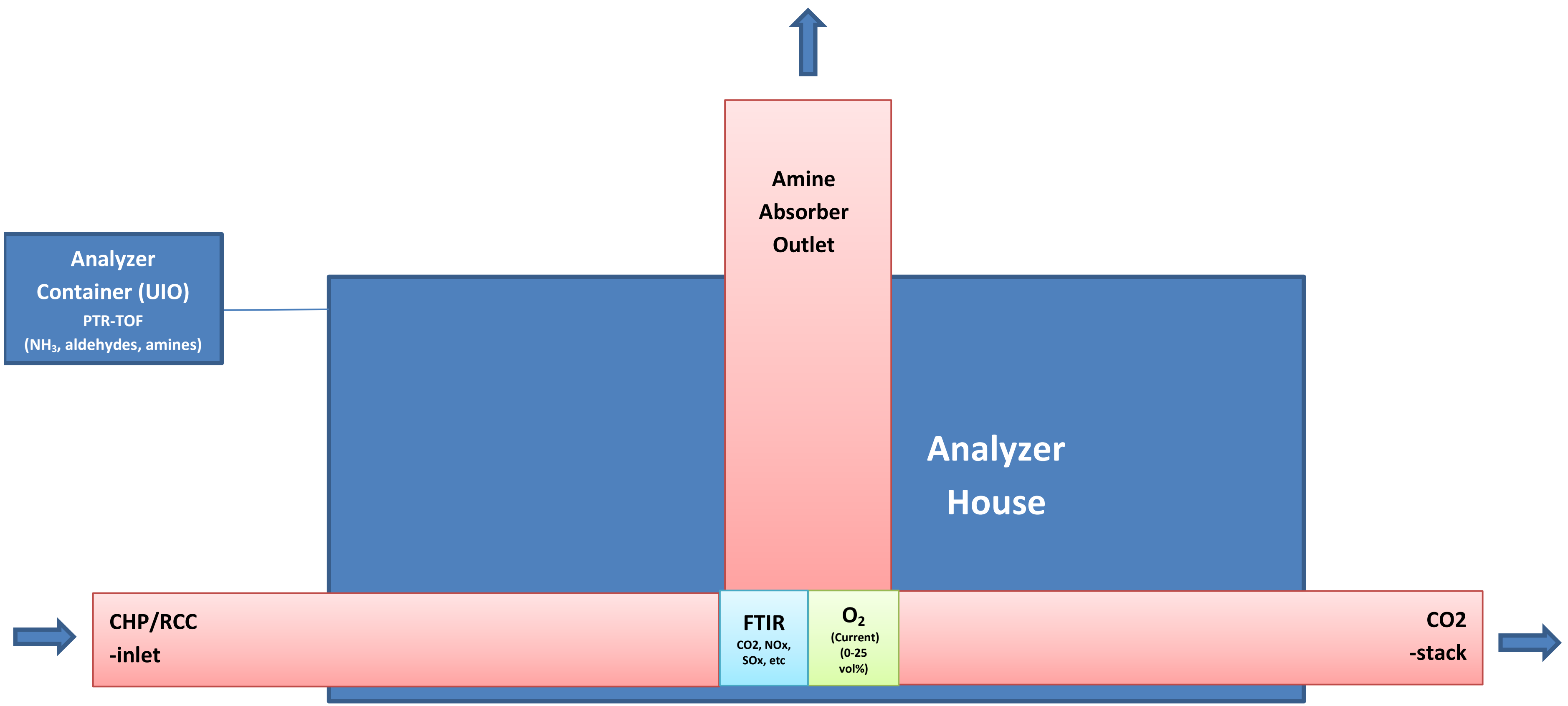
- Amine plant/absorber at TCM is suited for simulator verifications
  - Temperature and α_{CO2} loading profiles are essential → preferably also CO_2 gas phase profiles
- A simulator is a good tool for understanding mass transfer when compared to experimental data
  - Highest flux occurs in the middle of the absorber column, pinching to be avoided
  - Further model development essential
    - Mass transfer correlations
    - Higher MEA concentration ranges
  - Simulator temperature profile match is not sufficient for complete description of the mass transfer process
- Further testing necessary
  - Increased CO_2 flue gas content → RCC gas with 13-15% CO_2

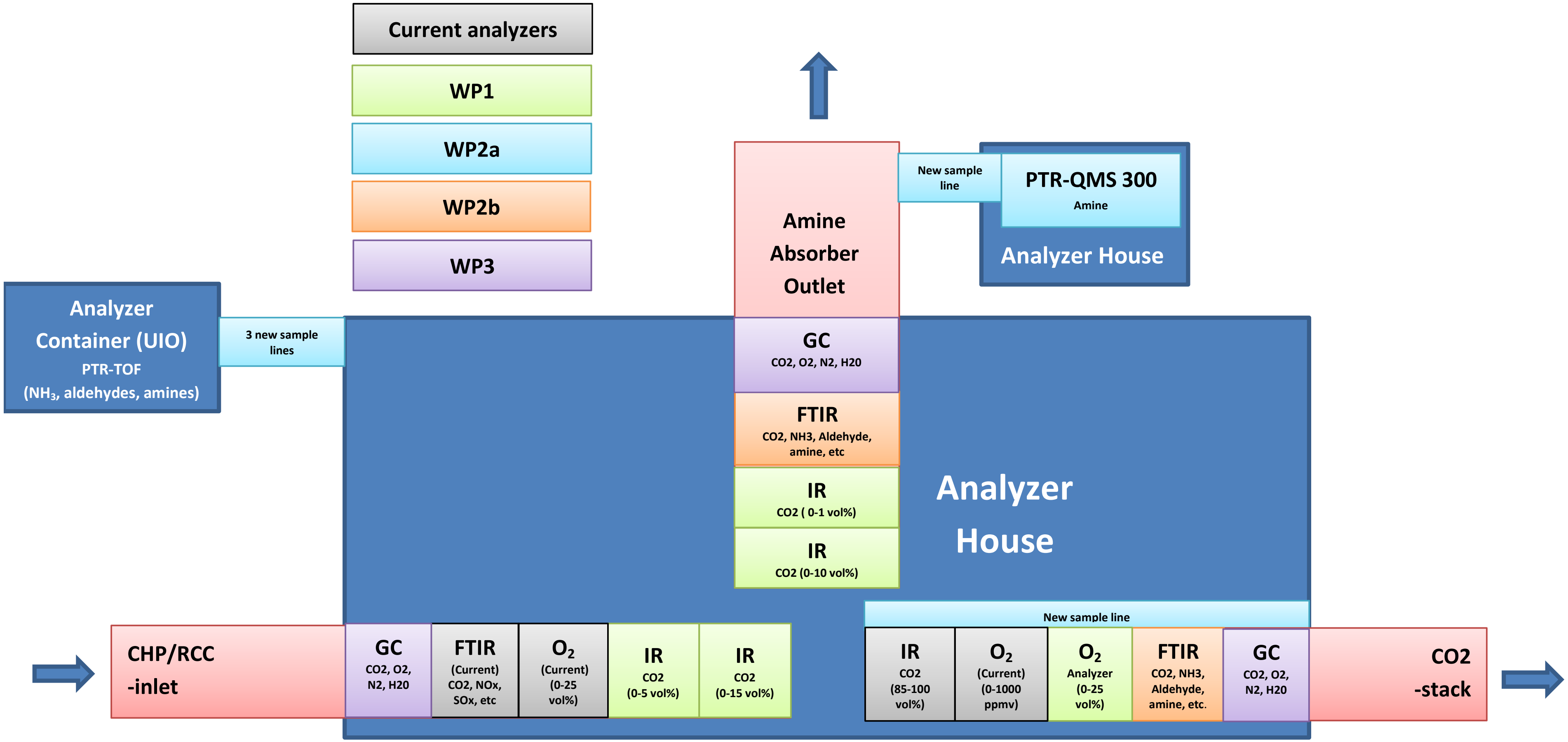
Thank you for your attention!!!

Questions???

Acknowledgments to TCM DA owners

GASSNOVA Statoil sasol reaching new frontiers


Amine
Absorber
Outlet
Analyzer
Container (UIO)
PTR-TOF
(NH3, aldehydes, amines)
Analyzer
House
CHP/RCC
-inlet
FTIR
CO2, NOx,
SOx, etc
O2
(Current)
(0-25
vol%)
CO2
-stack



Current analyzers
WP1
WP2a
WP2b
WP3
Analyzer Container (UIO)
PTR-TOF
(NH3, aldehydes, amines)
3 new sample lines
Amine Absorber Outlet
New sample line
PTR-QMS 300
Amine
Analyzer House
GC
CO2, O2, N2, H20
FTIR
CO2, NH3, Aldehyde, amine, etc
IR
CO2 (0-1 vol%)
IR
CO2 (0-10 vol%)
Analyzer House
CHP/RCC -inlet
GC
CO2, O2, N2, H20
FTIR
(Current) CO2, NOx, SOx, etc
O2
(Current) (0-25 vol%)
IR
CO2 (0-5 vol%)
IR
CO2 (0-15 vol%)
New sample line
IR
CO2 (85-100 vol%)
O2
(Current) (0-1000 ppmv)
O2
Analyzer (0-25 vol%)
FTIR
CO2, NH3, Aldehyde, amine, etc.
GC
CO2, O2, N2, H20
CO2 -stack