CAPE-OPEN Unit Operation for OGT Simulation Software

CAPE-OPEN 2019 Annual Meeting

Shell Technology Centre Amsterdam (STCA)

October 22-23, 2019

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Introduction

About OGT

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About OGT - Background

- Optimized Gas Treating, Inc. (OGT) est. 1992 by Ralph Weiland and Jack Dingman
  - Windows-based software package originally for simulating acid gas removal specifically with aqueous alkanolamines
    - Built on fundamentals of mass-transfer rate-based approach
    - Intuitive and simple – engineers focus on design
    - Predictive modeling - real Hardware information
      - Based on many years of research and development
        - 30 years of university research in gas treating
        - Physical Property and Mass Transfer correlations
          - Scheffe-Weiland etc.
        - Development of trays – flooding/choke correlations, SUPER-FRAC | ULTRA-FRAC | Kittel
  - First commercial software release in 2000

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About OGT - Background

- Simulation Common Ancestry
  - ProTreat®, RATEFRAC®, RateSep® - Weiland PhD work (1965-1968)
  - NSF/DOW/Ross Taylor/Ralph Weiland – Mainframe model (1982)
  - Koch/AspenTech (RATEFRAC) – Taylor and Weiland Acs. (GASPLANT)
    - RATEFRAC – Dr. M.S. Sivasubramanian – graduate student of Weiland
  - ChemShare Corp. (WinSim®) – bought rights to GASPLANT

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About OGT – What we do

OGT | ProTreat®

- Acid Gas removal applications
- Sour water stripping
- Rate-based glycol dehydration with Stahl columns
- Caustic mercaptan removal
- aMDEA LNG and ammonia
- TGTU, Quench, TGU Amine, AGR, AGE
- Corrosion predictions
- Vendor solvents and packings
- Fully flexible flowsheeting tool

OGT | SulphurPro®

- Reaction kinetics in the Reaction Furnace
  - COS & CS_2 formation kinetics
  - NH_3, BTEX & hydrocarbon destruction kinetics
- Waste heat boiler/Sulphur condenser sizing/rating and utility calculations
  - COS & H_2 recombination reactions
- COS and CS_2 destruction kinetics in Sulphur converters
- Dew Point/Conversion profiles across converter beds
- $H_2S/H_2S_X/SO_2$ solubility in liquid Sulphur streams
- SUPERCLAUS®, Sub-dew-point, COPE recycle

Consulting Services

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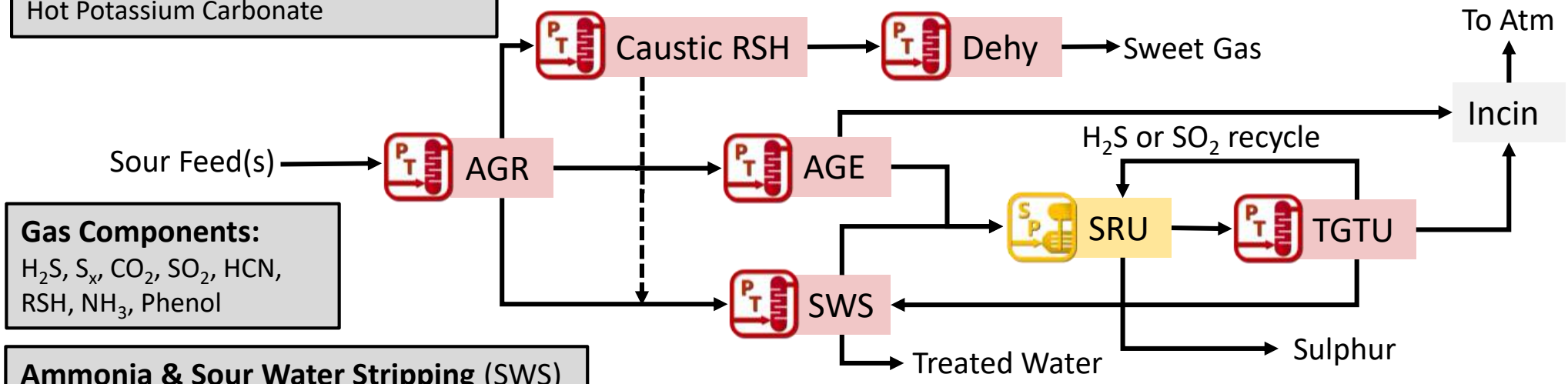
About OGT – What we simulate

Amine Units (AGR/AGE/TGTU)
All amines plus 2- & 3-amine blends
Accurate VLE & Transport Properties
Specialty Solvents: Ineos Gas/Spec, Dow Ucarsol, Eastman AdapT, Ion,
Heat Stable Salts & Stripping Promoter
Hot Potassium Carbonate

Dehydration Units: MEG, DEG, TEG

Physical Solvents: DMPEG (Coastal AGR®) (e.g. SELEXOL™)

Hydrocarbon, BTEX
solubility in Amines and Physical Solvents



Gas Components:
H_2S, S_x, CO_2, SO_2, HCN, RSH, NH_3, Phenol

Ammonia & Sour Water Stripping (SWS)
Accurately model SW ion species

H_2S/CO_2 wet corrosion prediction in amine and sour water systems

Caustic Treating
NaOH and KOH

Sulphur Recovery Units (SRU)
Kinetic and heat transfer rate for WHB, Reaction Furnace and Converters; Sulfur Condensers, accurate $SO_2/H_2S/S_x$ properties

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About OGT – What makes OGT unique

- Rate-based simulation
  - OGT built from years of experience developing rate-based mass transfer for complex, ionizing chemical solutions
  - Extended into kinetic modeling of catalyst beds and plug-flow reactors in SulphurPro model
  - Robust algorithm – close solvent loops, initialize without guessing profiles
- Software for Engineers, by Engineers
  - Strive to keep things simple and intuitive
    - Add input specs that allow an engineer to focus on the problem, not mindless normalization and conditioning inputs.
    - Clean interface – put in only what is required to give accurate results
  - Out of the box simulation
  - Proprietary solvent blends incorporated into software

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About OGT – Who we work with (Operators/Suppliers)

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About OGT – Who we work with (Eng./Consulting)

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Project Background

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Incentives for CAPE-OPEN

- Customer driven addition
  - More and more companies are requiring CAPE-OPEN compliance
- Expansion of Capabilities
  - Allows OGT's expertise be paired with others to expand into complete plant simulation
  - Higher order optimization tools
    - Solve optimization problems at the plant or sub-flowsheet level
    - Hook into multivariable solver programs
  - Enable more efficient data transfer with less user-error

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Implementation of CAPE-OPEN Unit Operation

- Technical Notes
  - Implementation is COM based as internal infrastructure depends on COM
  - Support for both v1.0 and v1.1 thermodynamics
  - Support for energy streams (generic, thermal-, and axis-)
  - Support for parameter common interface and dimensionality
  - Support for reporting interface
  - Persistence support IPersistStream and IPersistPropertyBag
  - Support for interruption of calculations via named value “AbortCalculation”
  - Able to obtain list of compounds via Material Template System prior to connecting streams

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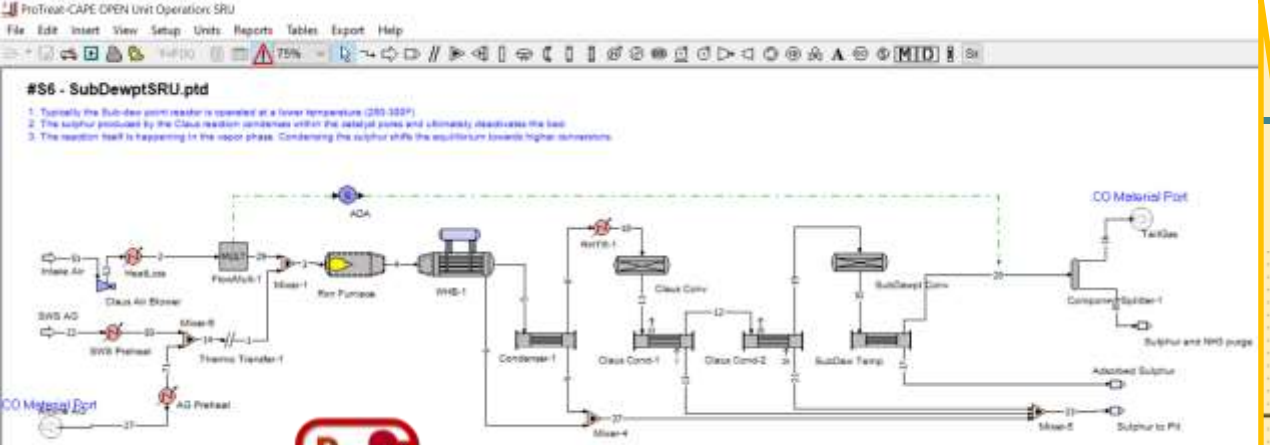
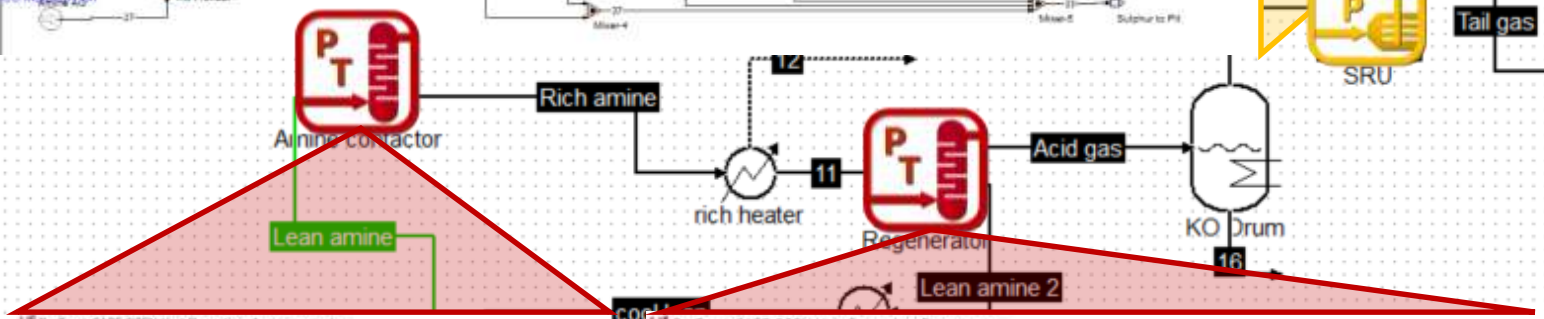
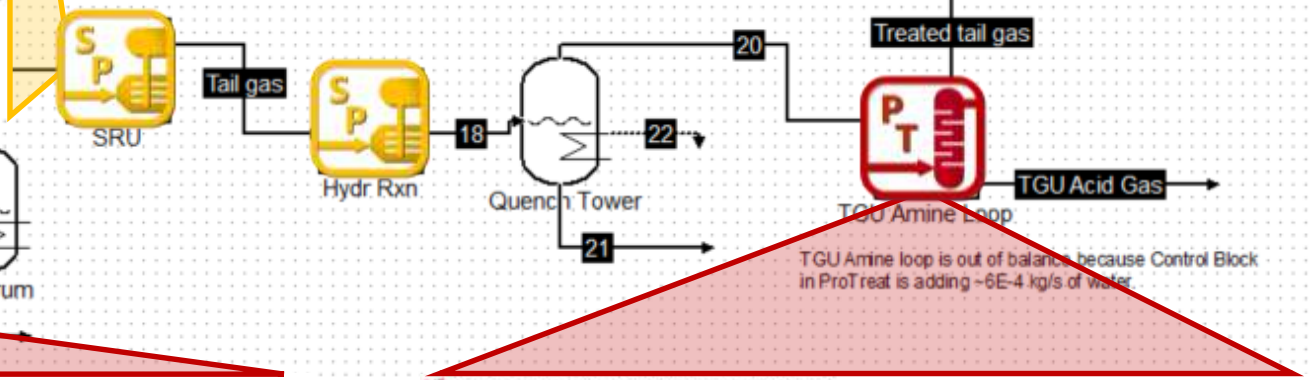
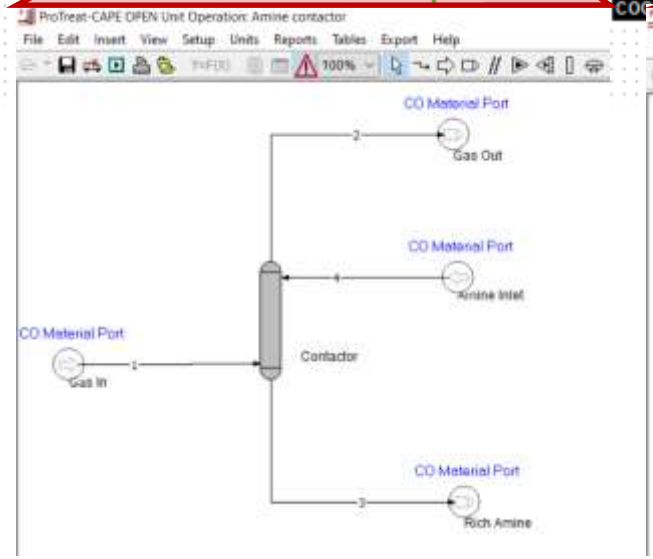
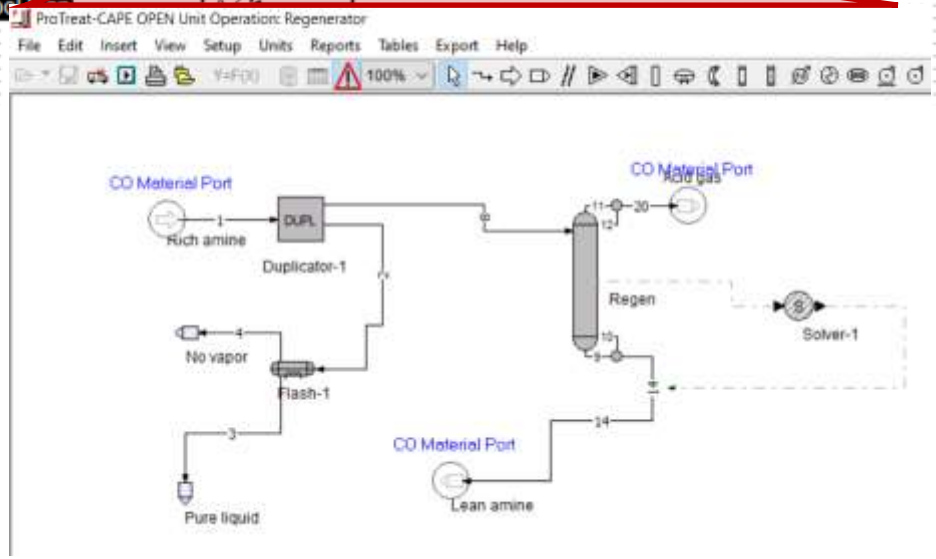
(Amine Treating/SRU)

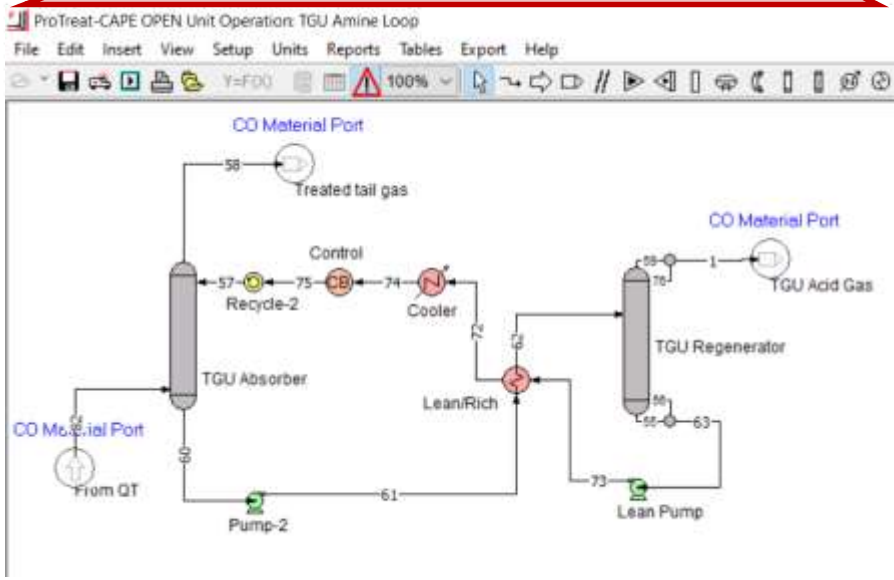












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CAPE-OPEN Demonstration

PRO/II Engineering 10.2 | ProTreat® v6.5.1

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CAPE-OPEN Demonstration

Honeywell UniSim® Design | ProTreat® v6.5.1

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Opportunities for CAPE-OPEN

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Realized Opportunities

- Customer interoperability
  - Expand range of use of software
  - Improve data import/export
- Expand software's range of use
- Direct Applications
  - SRU Catalytic Converter
  - Mass-Transfer absorber
  - …
- Peripheral Benefits
  - Improved internal tools – refactoring
    - Consulting projects and reports
    - Improved development speed

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Summary

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Summary

- CAPE-OPEN PMC implemented in OGT Software Suite
  - Successful demonstrations – UniSim, ProII, COFE
  - Still testing
    - Several Beta testers interested
- Benefits of CAPE-OPEN
  - Direct applications
  - Internal tool development and optimization

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Acknowledgements

- Thanks to AVEVA for the use of PRO/II Engineering 10.2 demo
  - For information on this product please see www.aveva.com

- Thanks to Honeywell for the use of UniSim Design demo
  - For information on this product please see www.honeywellprocess.com

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Thank you

Questions?

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OGT Inc.

Process Simulation Software

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