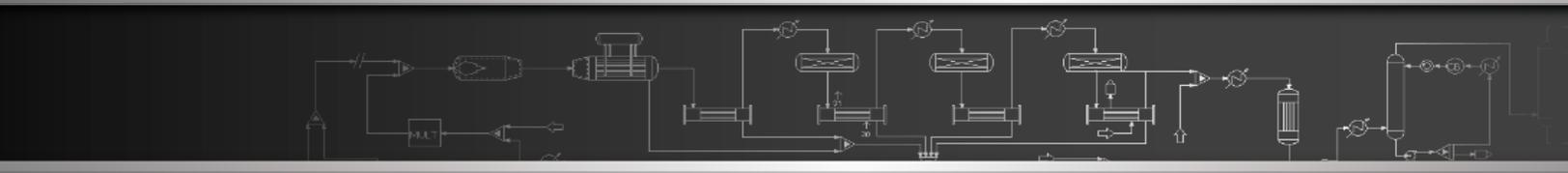




**OGT** Inc.

Process Simulation Software  
& Consulting Services



**Technical Brochure**

# Simulation for the 21<sup>st</sup> Century

- Advanced technology at affordable prices
- Trim the fat with tighter, more certain designs
- Customizable license – buy only the capabilities you use



## ProTreat<sup>®</sup>:

- The only accurate way to simulate packing
- Replace experience with actual data: NO HETPs, NO HTUs, no EFFICIENCIES
- Improve selectivity using the spray regime on trays
- The simulator with the most branded specialty solvents
- Account for heat stable salts & degradation products
- Sour Water Stripping including WWT
- Rate-based glycol dehydration and physical solvent treating with real Stahl columns
- Caustic treating to remove mercaptans
- Piperazine promoted MDEA in hydrogen, LNG, and Ammonia
- TGTU, Quench, TGU Amine, AGR, AGE
- Effect of SO<sub>2</sub> on TGTU Quench and Tail Gas Amine systems
- Predict corrosion rates
- Unique carbon capture solvents (Alkazids, enzyme catalysts)
- All acid gas removal applications seamlessly integrated with ...



## SulphurPro<sup>®</sup>:

- Reaction kinetics in the Reaction Furnace
  - COS & CS<sub>2</sub> formation kinetics
  - NH<sub>3</sub>, BTEX & hydrocarbon destruction kinetics
- Waste heat boiler/Sulphur condenser sizing/rating and utility calculations including recombination kinetics
  - COS & H<sub>2</sub> recombination reactions
- COS and CS<sub>2</sub> destruction kinetics in Sulphur converters
- Dew Point/Conversion profiles across converter beds
- H<sub>2</sub>S/H<sub>2</sub>S<sub>x</sub>/SO<sub>2</sub> solubility in liquid Sulphur streams
- SUPERCLAUS<sup>®</sup>, Sub-dew-point, oxygen enrichment, COPE<sup>®</sup> recycle, double combustion



# ProTreat<sup>®</sup>: Modern Software for Gas Treating Simulation

You expect the right answers – ProTreat delivers them

## Benefits

- Reliable answers at an affordable price
- Customizable license – you only pay for what you need
- State-of-the-art mass transfer rate-based modeling
- Robust, fast, versatile, intuitive, uncluttered
- Ready out-of-the-box
- Learning curve: Hours, not days

## ProTreat<sup>®</sup> is Number One for Simulation Of:

- Piperazine promoted MDEA for H<sub>2</sub>, LNG, & Ammonia Production
- Selective H<sub>2</sub>S removal
- Acid Gas Enrichment
- Caustic Treating, Dehydration, Sour Water Stripping
- Accurate performance of random and structured packings
- Sulphur Recovery Units fully integrated with gas treating
- TGTUs & Quench towers
- Corrosion rate prediction

## Proprietary and Specialty Solvents:

- |                       |                        |
|-----------------------|------------------------|
| 1. INEOS GAS/SPEC*    | 7. Dow UCARSOL™        |
| 2. Eastman AdapT®     | 8. Amino Acids         |
| 3. CCS Solvents       | 9. PZ Promoted MDEA    |
| 4. Enzyme Catalysts   | 10. Clariant Genosorb® |
| 5. FLEXSORB® SE /Plus | 11. DEG®, ADEG®        |
| 6. Coastal AGR®       |                        |

## Technical Support:

- Fast, Responsive, Comprehensive
- E: [support@ogtrt.com](mailto:support@ogtrt.com) | P: +1 512 312 9424



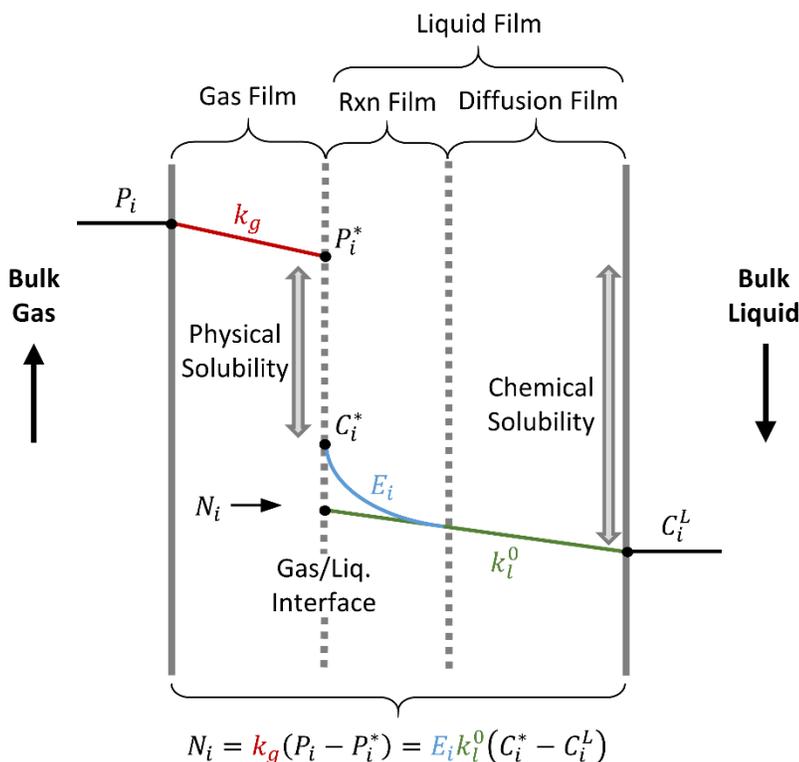
# Equilibrium Stages vs. Mass Transfer Rate Modeling

Proven, predictive, fundamental design.

**R**igorous, mass transfer rates are used for all column calculations by ProTreat<sup>®</sup>, eliminating the need for empirical adjustments to simulate new applications correctly. The ProTreat mass transfer model is built on five key elements:

- Mass and energy balances around individual phases on a tray or packed segment
- Activity-based thermodynamic phase equilibrium including a rigorous non-ideal aqueous electrolyte model incorporating chemical reactions
- Equilibrium across the phase boundary
- Chemical kinetics effects on mass transfer rates
- Mass and heat transfer rate models for transport of critical components (including water) and energy across the phase boundary

In contrast, even the most sophisticated equilibrium stage model uses only two of these elements, namely mass and energy balances around an entire ideal stage plus thermodynamic phase equilibrium.

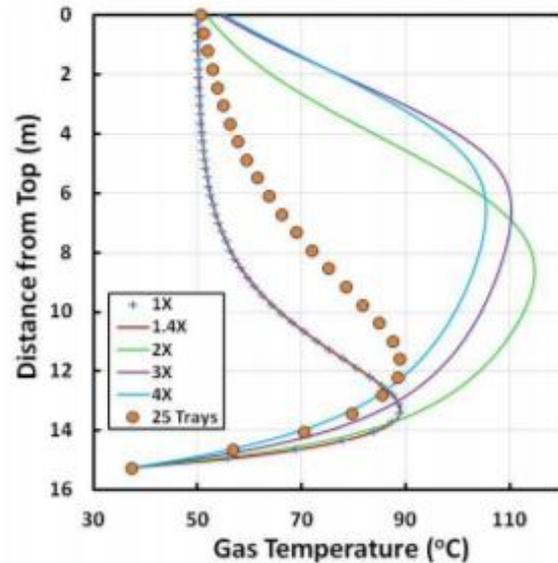
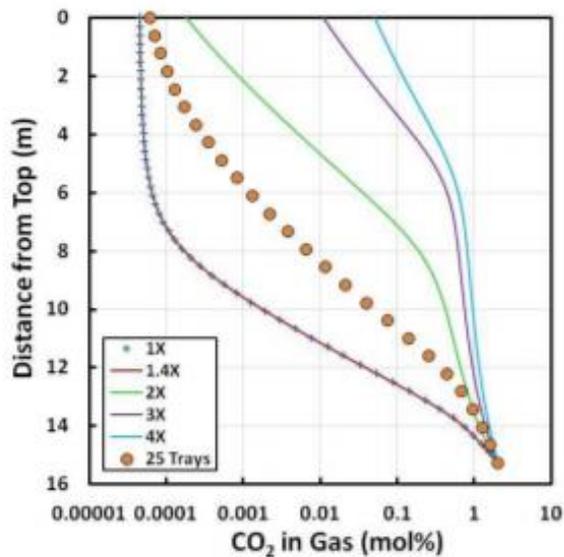


In a mass transfer rate model, there are intricate interrelated effects between the five key elements. They respond by a variety of chemical and physical, phase and component transport properties such as:

- Chemical kinetics
- Diffusion coefficients
- Solvent viscosity and other transport properties
- Salting-out effects on solubilities
- Mass transfer characteristics of the actual hardware being used.

When a ProTreat column simulation is run, the tower is being modeled in full detail as a piece of real equipment, not as an idealization.

Equilibrium stage simulators often attempt to include reaction kinetics by empirical modeling via an adjustable parameter (H<sub>2</sub>S and CO<sub>2</sub> tray efficiencies and/or liquid residence times) that forces the simulation to reproduce a conventionally-operated column's treated gas composition. In reality, separation efficiencies are complex functions of the chemical system as well as the column internals: specifying an efficiency makes a model **nonpredictive**. Equilibrium models are unable to deal with applications dependent on differences between mass transfer rates of CO<sub>2</sub> and H<sub>2</sub>S for which operating experience is lacking.



From a separations standpoint, two-pass and single-pass trays perform differently. Metal packing gives different results from plastics and ceramics. In addition, all solvent properties, including the changes in these properties caused by acid gas loading, affect mass transfer coefficients and thereby influence the actual separation that a given column under a given set of operating conditions will achieve.

ProTreat's mass transfer rate model is rich in detail and is a faithful mirror of the real world. In the language of process control, a true mass transfer rate simulation uses a distributed parameter model that, consequently is mechanistic, detailed, and fully predictive. This is in contrast to the equilibrium stage approach which is a lumped parameter model - it assigns all the physical and chemical complexities to an efficiency or a liquid residence time and is accordingly completely nonpredictive.

ProTreat is the only simulator that allows you to *predict* packed tower *mass transfer* performance, not just hydraulic rating. Proven, fundamental mass transfer performance information is available for 24 types of random and 7 types of structured packing from all major packing suppliers. If the packing you want to use isn't in ProTreat, we'll add it in for you.

Mass transfer performance predictions have been validated against a large amount of full-scale plant performance data, and regeneration columns are simulated just as accurately as absorbers. ProTreat is 100% mass transfer rate-based and uses detailed chemistry and mass transfer calculations to predict performance of real equipment without guesswork.



# LNG Facilities

## Simulation for Initial Design, Revamps, Optimization, and Troubleshooting

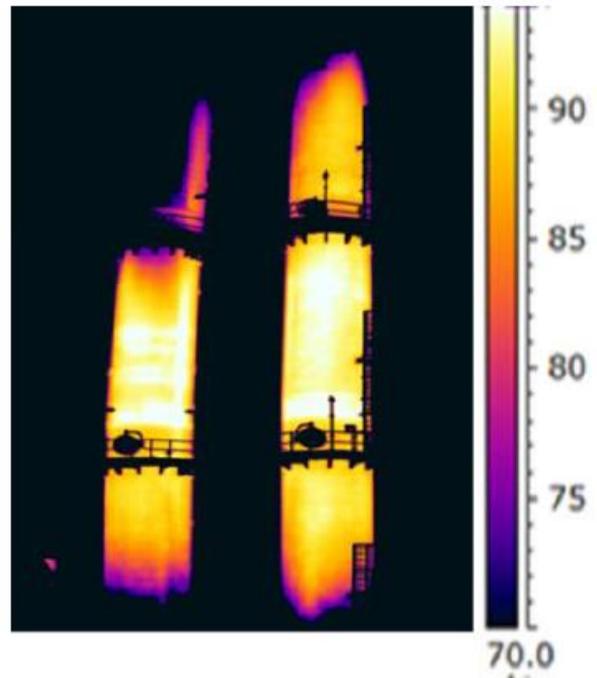
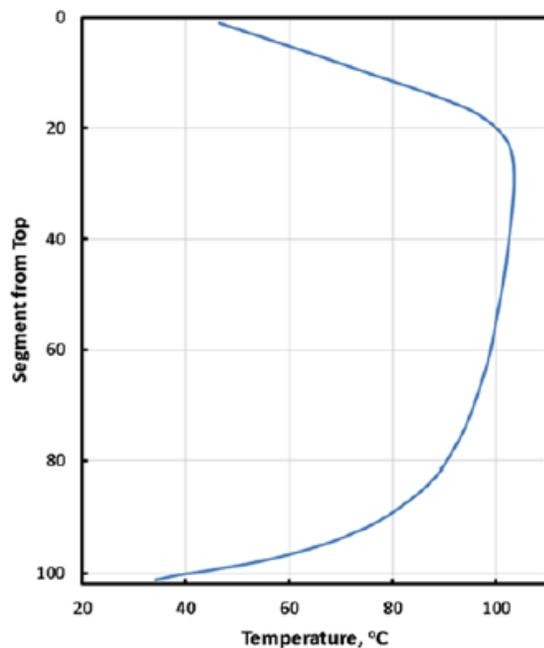
**P**roTreat® is the only commercially available simulator consistently proven in LNG applications using piperazine promoted MDEA solvents as well as DGA® and ADEG® for CO<sub>2</sub> removal. ProTreat has been 100% mass transfer rate based since inception.

ProTreat has been tested in designing and troubleshooting AGRUs in large scale LNG plants around the world, from Australia to Alaska to Africa and offers unprecedented reliability, accuracy, and predictive power. Get answers you can trust

### A Recent Troubleshoot

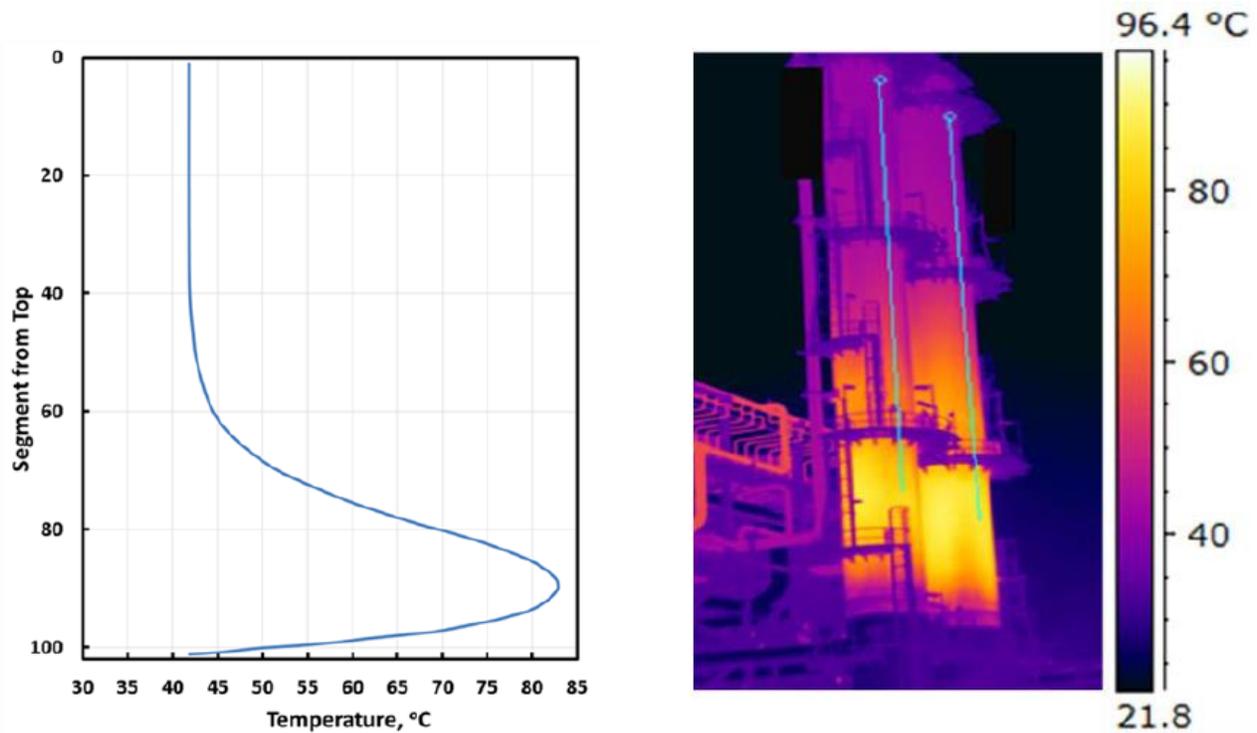
#### The Case Before

In a recent troubleshoot of one of the AGRUs in a very large scale, multi-train LNG plant, the two parallel absorbers were found to be running extremely hot, although still meeting the < 50 ppmv CO<sub>2</sub> specification. The temperature profile predicted by ProTreat is compared with a thermal image here...



#### The Case After

With measured outside skin temperatures approaching 100°C there were concerns about serious corrosion in the upper parts of these absorbers, where there was no stainless cladding. The absorbers were running with less than 75% of the design solvent flow (piperazine + MDEA). After increasing the solvent flow to a value closer to the design rate, the absorbers operated with temperatures profiles shown here...



The bulge temperature was still warm (80–85°C) but the peak was in the bottom part of the towers where they are stainless steel clad so there are no corrosion concerns. Incidentally, the measured and simulated CO<sub>2</sub> levels in the treated gas were 2 ppmv and 1 ppmv, respectively.

ProTreat has the remarkable ability to predict performance consistently and with uncanny accuracy, using only information you can read from equipment drawings and spec sheets. Mellapak Type-X structured packing was used in the columns shown here. Other cases have used other structured packings, as well as random packings such as Raschig SuperRings®.

LNG plants are very costly to build and operate. ProTreat removes unnecessary risks associated with guessing HETPs and tray efficiencies and producing a suboptimal design or, worse, a design that just doesn't work, requiring a very difficult and expensive revamp. If you're going to simulate the performance of structured and random packing reliably in this application, there is absolutely no substitute for a real mass transfer rate-based simulator.



# Predict Performance of Real Solvents

Amines are clean only on the day they are charged to the systems –  
Real Solvents are contaminated



Amine solvents are often contaminated with **heat stable salts** (HSSs), **alkali metals** such as sodium and potassium, plus other **degradation products** including other amines not originally present in the solvent. Contaminants can have a profound effect on how well the solvent performs in a given application, and on its corrosivity.

Sometimes a contaminant is deliberately added to a solvent to promote regeneration. For example, phosphoric acid is a HSS that is purposely added to enhance the regenerability of MDEA. HSSs that are produced in refinery amine systems can enhance regeneration as well. However they can make it either harder or easier to remove  $H_2S$  to very low levels—circumstances dictate.

DEA and MMEA are products of MDEA degradation that can seriously affect the selectivity of MDEA for  $H_2S$ , especially in TGTUs and AGEs.

The true effect of contaminants depends on which specific ones are present and in what concentrations, as well as on the operating conditions of the units themselves. **Design and predict the performance of end-of-run (EOR) conditions for degraded, HSS laden solvents.**

ProTreat® is the only commercially available simulator that accounts for the incomplete dissociation of a wide range of individual heat stable salts (HSSs). You don't have to try to convert your solvent analysis into a phosphoric acid pseudo-equivalent. Each HSS dissociates differently (and incompletely) in a unique way. ProTreat also accounts for the serious reduction in selectivity caused by alkali metals, as well as by DEA and highly reactive MMEA in MDEA-based solvents.

**Optimize your design and build a plant you  
can be certain will perform as expected.**

# Carbon Capture and Sequestration

## Simulate carbon capture with CCS-specific solvents

**P**ost-combustion carbon capture's objective is to remove CO<sub>2</sub> with minimal regeneration energy. ProTreat® lets you simulate complex, highly heat-integrated flow sheets for CO<sub>2</sub> capture using all the standard amine solvents and their blends, plus:

- AMP (2-amino-1-methyl propanol)
- Sodium glycinate (an amino acid)
- Solvents promoted with enzymes such as carbonic anhydrase
- High strength piperazine

Gas liquid contacting in absorption columns is the most common proposal. Huge volumes of low-pressure gas need towers with the lowest pressure drop possible – perfect for structured packing.

ProTreat is the only simulator that allows you to *predict* packed tower *mass transfer* performance, not just hydraulic rating. Proven, fundamental mass transfer performance information is available for 24 types of random and 7 types of structured packing from all major packing suppliers. If the packing you want to use isn't in ProTreat, we'll add it in for you.

Mass transfer performance predictions have been validated against a large amount of full-scale plant performance data, and regeneration columns are simulated just as accurately as absorbers. ProTreat is 100% mass transfer rate-based and uses detailed chemistry and mass transfer calculations to predict performance of real equipment without guesswork.



# Tail Gas Treating

**Predict selective absorption – No HETPs, HTUs, or Efficiencies Required**

**T**reating the tail gas from an SRU aims to minimize H<sub>2</sub>S leak to incineration and minimize the CO<sub>2</sub> recycled to the SRU by maximizing CO<sub>2</sub> rejection. Because TGU absorbers handle very low-pressure gas, they usually contain either random or structured packing to minimize pressure drop. With ProTreat®, estimating HTU or HETP values is no longer necessary, and design is more certain. ProTreat knows how your column internals work. ProTreat uses a rate-based model and the characteristics of the tower's real internals to calculate directly not just hydraulic performance but the separation performance in terms of H<sub>2</sub>S leak, CO<sub>2</sub> slip, plus detailed maps of how composition and temperature are changing inside the bed. Simulate 31 types of random and structured packings in all the available sizes, and with hydraulics that match supplier data.

MDEA and phosphoric-acid-promoted MDEA are the solvents of choice for TGTUs. However, the gas from an SRU quench column often contains SO<sub>2</sub> which degrades MDEA into DEA and MMEA. Both react with CO<sub>2</sub>, with MMEA reacting faster than any other gas treating amine except piperazine. MMEA is an activator of MDEA with the result being a very significant loss of selectivity. H<sub>2</sub>S leak to the incinerator can increase by 10 or 20 times compared to clean solvent, and the load on the SRU will go up because of excessive CO<sub>2</sub> recycle from the tail gas. ProTreat very precisely simulates TGTUs with degraded amine solvent, it allows for the effect of HSSs formed from HCN and other contaminants, and it accounts accurately for the benefit that can be realized by using the stripping promoter phosphoric acid or in-situ heat stable salts from SO<sub>2</sub> breakthroughs.

**Unit Engineers Deal with Reality:  
Shouldn't your simulator?**



# Glycol Dehydration

## Property and Internals Dependent, Predictive Mass Transfer



**G**lycol dehydration isn't quite as simple as it looks. There are at least four factors that recommend the ProTreat® mass transfer rate-based approach:

- Glycol is highly viscous, especially when very dry – similar to peanut or soybean oils. Viscous fluids resist absorption. HETP “rules” are based on water-like liquids, not viscous fluids.
- Resistance to absorption and stripping can change from gas to liquid phase across the height of both the absorber and regenerators, making it tough to estimate HETPs and efficiencies.
- Stahl columns can get you 99.8+ wt % glycol but they aren't ideal stages. Stripping depends on tower internals and with ideal stages it's impossible to provide more than a very rough estimate with a stripping gas.
- Dehydration columns today use structured packing rather than trays. Packing is beyond the ability of most engineers to come up with reliable figures for HETP values.

ProTreat's rate-based model replaces personal experience with a large database of fundamental phase, flow, and property dependent parameters to calculate mass transfer coefficients. The huge uncertainty of always-limited experience and the resulting necessity for oversized systems is replaced with more certain, optimized designs at a price so small, it vanishes into any budget.

**Optimize your design and build a plant you can be certain will perform as expected.**

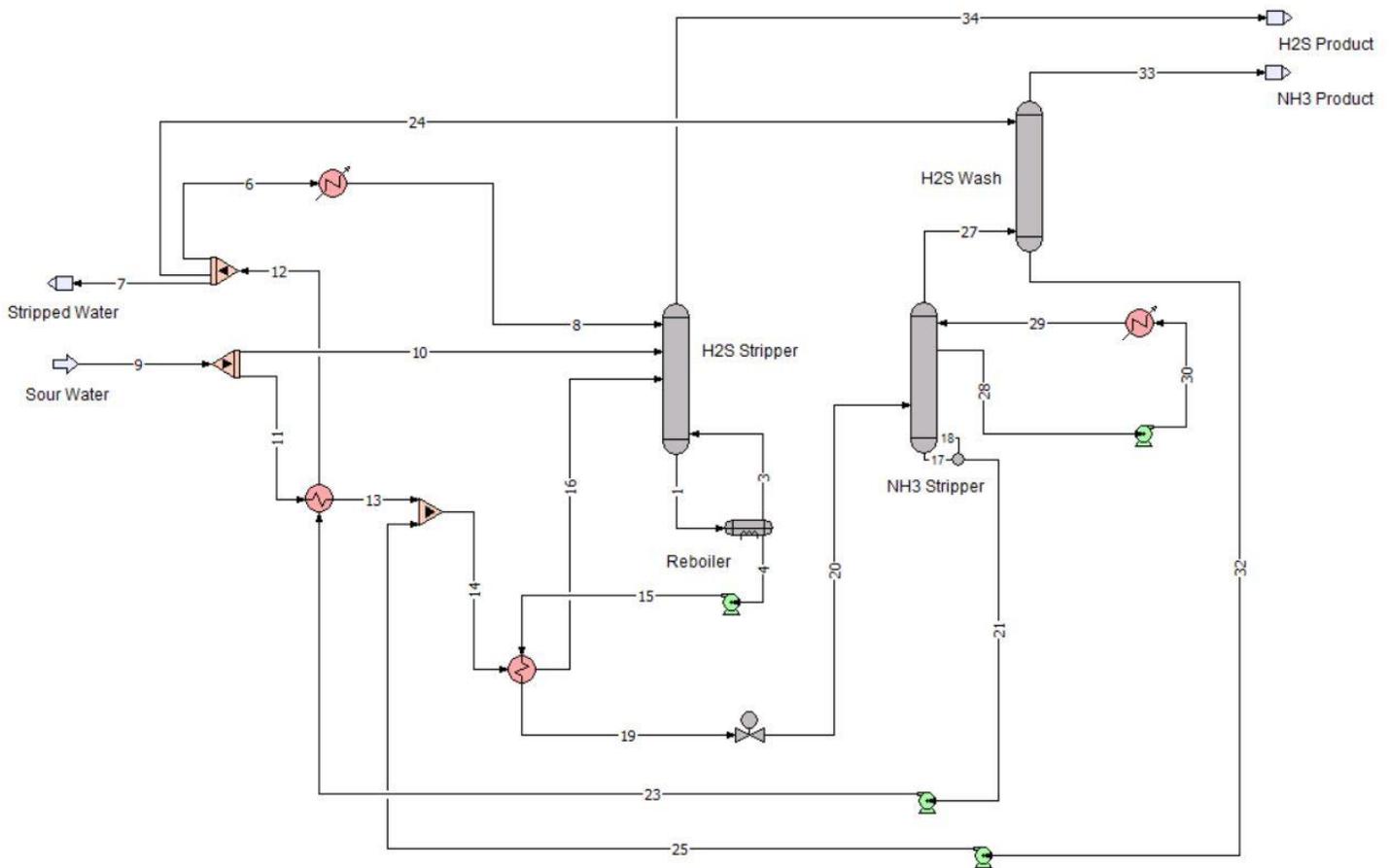
# Sour Water Stripping

Account for ALL factors

Sour water stripping is fraught with numerous issues other simulators ignore or fall short on:

- Limitations caused by refinery heat stable salts
- Caustic injection to neutralize contaminants
- Modeling special process configurations such as Chevron WWT technology
- Predicting where ammonia hangs up in strippers
- Account for HCN and phenols

With rate-based simulation, ProTreat® does it all. Get the right answers every time.



## Chevron Waste Water Treatment (WWT) Process

# Quench Towers

## Mass transfer limits in a “heat transfer” device



A quench tower is a cooling tower that achieves liquid or gas cooling by direct contact between the phases. Cooling results from evaporative or transpiration cooling as well as by sensible heat transfer. In a quench tower, some of the liquid vaporizes and transfers the heat associated with sensible cooling into latent heat of vaporization. This is a form of humidification operation which, in engineering, is recognized as a fairly difficult calculation to make.

Quench towers may be spray-type devices but usually they contain internals. The internals are always packing, either a very large crimp structured type of packing or very large random packing such as Raschig Rings. This is called film contact because the liquid runs over the packing as a film. Alternatively, splash contacting can be done using a drip grid type of packing.

ProTreat® is extremely well suited to simulating quench towers because of its strict mass and heat transfer rate basis. In a TGU Quench tower, hot gas from hydrogenation is directly contacted with the cooling water running over the packing. The cooling rate is actually controlled by water evaporation and condensation rates—sensible heat transfer plays a relatively minor role. In fact, water evaporation and condensation rates are controlled by the gas-phase resistance to the transfer of water between the gas and the water surface. Evaporation occurs in the tower bottom section while water condensation takes place in the top. Ammonia and SO<sub>2</sub> slip can be accurately modeled to predict sour water bleed disposition, solution pH, and contaminants slip into the downstream amine system.

ProTreat models the process using gas and liquid resistances to mass and heat transfer together with the interfacial contact area. These quantities are unique to the packing type, size, and material, allowing ProTreat to predict quench tower performance with high level of accuracy.

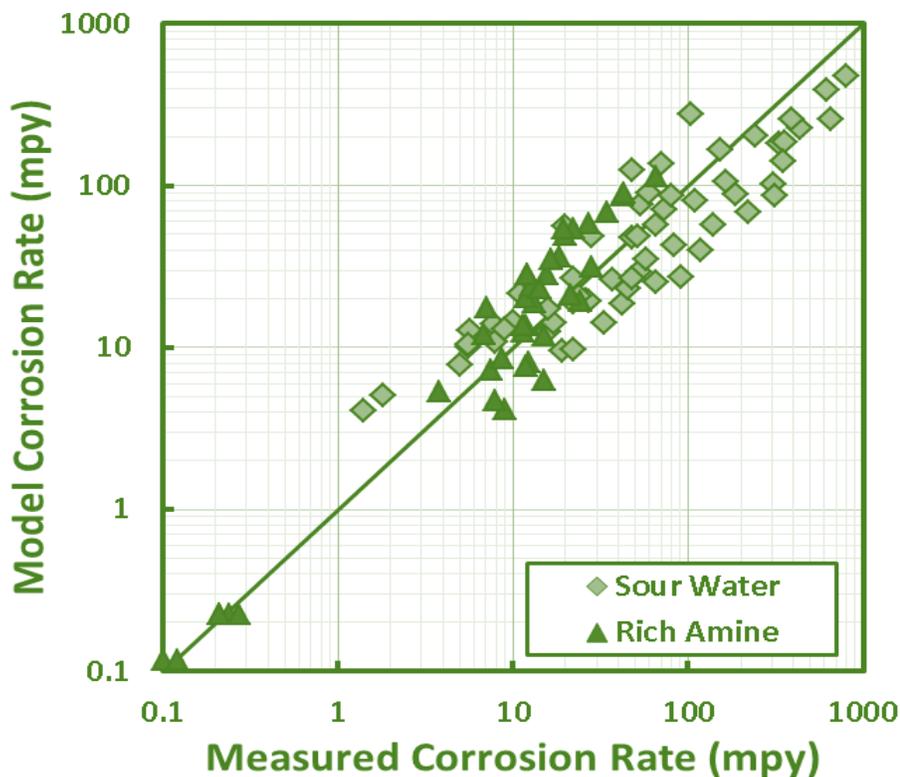
**Optimize your design and build a plant you can be certain will perform as expected.**

# Acid Gas Corrosion

Predict corrosion rates in acid gas systems with various metallurgies

**P**roTreat® offers a detailed chemistry and hydraulics-based predictive corrosion model built on both public and proprietary corrosion rate data. In the model, chemical species of interest are: bisulphide ion ( $\text{HS}^-$ ), physically dissolved  $\text{H}_2\text{S}$ , bicarbonate ion ( $\text{HCO}_3^-$ ), and physically dissolved  $\text{CO}_2$ , all of which are oxidizing agents. The final distribution of molecular and ionic species is found by solving the equations of chemical reaction equilibria, atom balances, and a charge balance to determine the solution's speciation.

ProTreat's model calculations are based on activity-based solution speciation, fluid velocity, pipe roughness, type of fitting (elbows, tees, etc.), temperature, and the type of metallurgy (carbon steel, 304L, 316L, Alloys 2205, 2507, 825, C-276) using data for acid-gas loaded MEA, DEA, MDEA and sour water. Corrosion coupons can monitor any flowsheet liquid or two-phase stream.

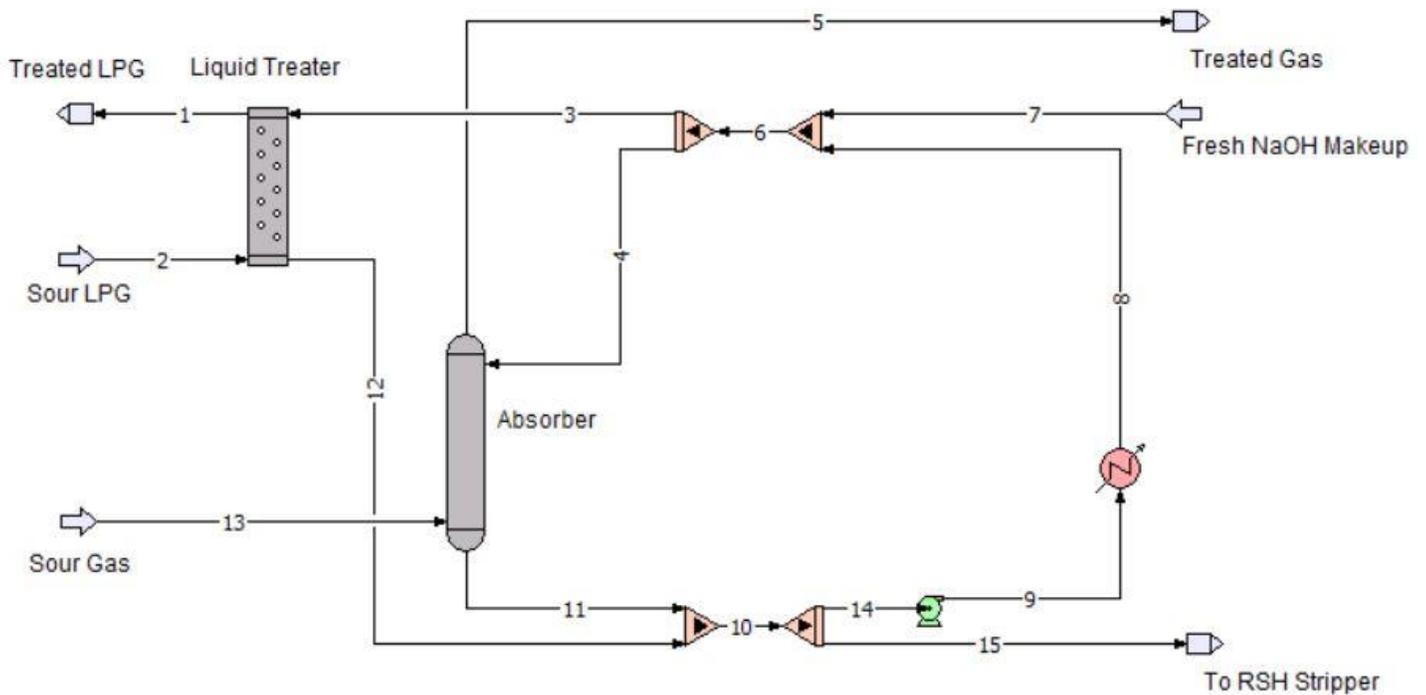


# Caustic Treaters

## Simulate organic Sulphur removal from gas and liquid products

Caustic units for removing mercaptans and other organic forms of sulphur from liquid and gas product streams are common in refineries. Usually the feeds have been pretreated with an amine to remove  $H_2S$  and any  $CO_2$ . The process is often a caustic bleed and feed system as seen here.

The physical solubility of organic sulphur in aqueous systems is quite low, and it is this low solubility that controls their absorption rate. ProTreat<sup>®</sup> uses a strict mass transfer rate basis to directly calculate absorption without ideal stages and their HTU and HETP accomplices. As a result, for a given tower and set of internals, the actual treated product composition is very accurately predicted. And when  $H_2S$  and  $CO_2$  are absent, not only can caustic regeneration using a reboiled stripper be done, it can be very accurately simulated, too.



## Caustic Feed and Bleed for RSH Removal

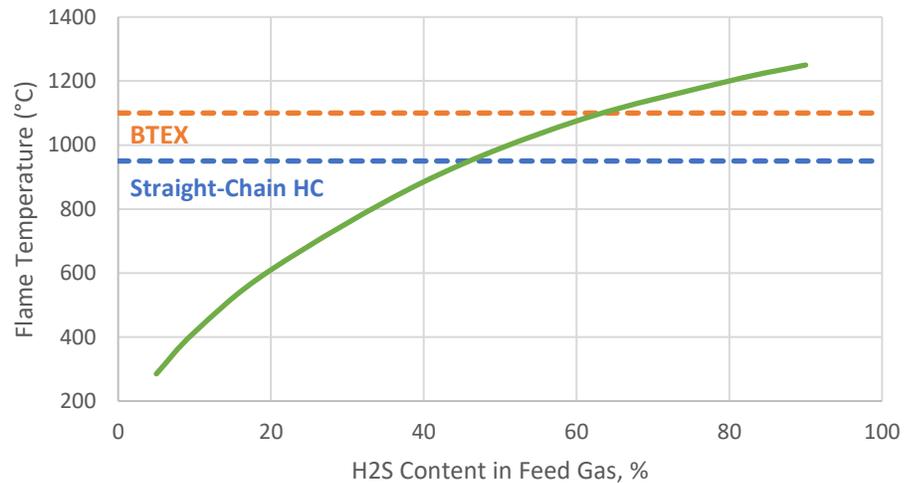
# Acid Gas Enrichment

Accurately predict selectivity by rate-based mass transfer



**A**cid gas enrichment (AGE) is challenging to simulate and design reliably — unless you're using ProTreat®, that is.

AGE depends critically on selectivity. The gas is mostly H<sub>2</sub>S and CO<sub>2</sub>. Both gases can be absorbed by the solvent so **AGE is the ultimate test for selectivity** — absorb as much H<sub>2</sub>S as possible, and slip as much CO<sub>2</sub> as possible when these are essentially the only species present. Get optimal SRU furnace operation and ensure destruction of hydrocarbons and BTEX components in the furnace.



AGE is usually a clean process because the feed gas has already been treated — it's the low pressure off-gas from an upstream amine unit. Packing is a good choice for an AGE absorption column because its large contact area per unit packing volume for an absorber of minimal size.

ProTreat is the only gas treating simulator capable of predicting the mass transfer (and hydraulic) performance of structured packing. Because it is truly mass transfer rate based and uses the actual mass transfer characteristics of the real internals, it gets enrichment and the H<sub>2</sub>S leak both exactly right.

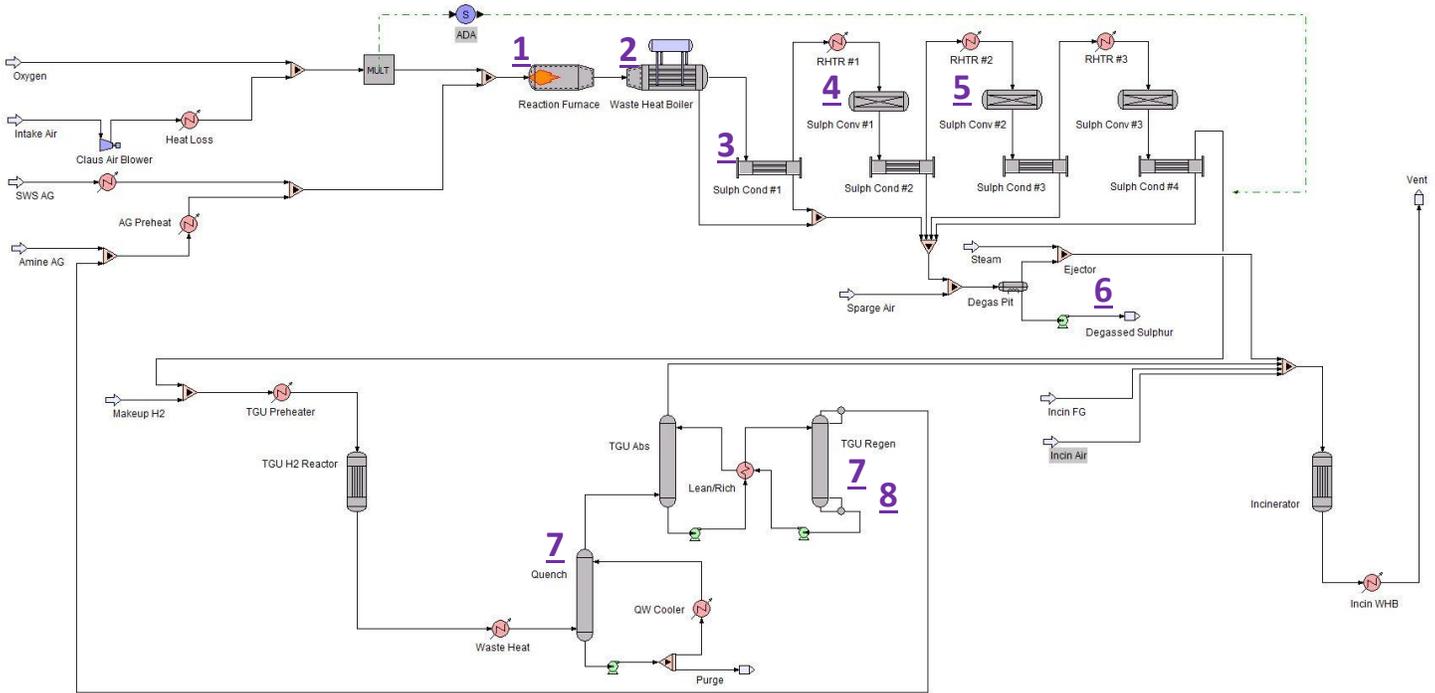
Predict the enriched gas composition, ensure H<sub>2</sub>S in the gas-to-flare meets sulphur emission standards, and maximize sulphur in the gas to the SRU by slipping as much CO<sub>2</sub> as possible. Do all this with MDEA, or proprietary solvents, or use stripping promoters to get an even cleaner stack gas.





# SulphurPro<sup>®</sup>: Sulphur Recovery Units

Simulate Sulphur recovery integrated with AGRs, AGEs, SWSs & TGUs



## Model with SulphurPro<sup>®</sup>:

1. Kinetics of COS & CS<sub>2</sub> formation & NH<sub>3</sub> + BTEX + Hydrocarbon destruction
2. Waste Heat Boiler sizing/rating and utility calculations including kinetics of COS formation and H<sub>2</sub> recombination that impact heat flux at the critical tube-to-tubesheet joint – a common reliability failure point
3. Rigorous Sizing/Rating integrated with simulation of Sulphur condensers
4. Claus catalyst activity with accurate COS, CS<sub>2</sub> hydrolysis & Sulphur dew point profiles across converter beds
5. Fix or predict conversion + predict COS & CS<sub>2</sub> destruction kinetics in converters
6. Accurate predictions of H<sub>2</sub>S/H<sub>2</sub>S<sub>x</sub>/SO<sub>2</sub> solubility in molten Sulphur and physical properties including the Sulphur pit
7. The effect of SO<sub>2</sub> on TGTU Quench and Tail Gas Amine Systems
8. The effect of HSSs & MMEA on Tail Gas Amine Unit End-of-Run Performance

# Additional Resources

## Seminars:

- Gas treating and Sulphur recovery concepts and hands-on training
- Learn how you can efficiently and effectively use our software to meet your needs

## The Contactor™:

- Monthly technical newsletter
- Distributed to over 25,000 engineers and counting

## ProTips™:

- Monthly technical newsletter covering software-specific features
- Tips and guidance on unlocking the full power of simulation tools

## Publications:

- Categorized, searchable collection of our journal and proceeding papers

## TextBook:

- Advanced Gas Treating: The Engineering Science
  - Weiland, RH, Hatcher, NA (2012)
  - For process engineers, especially engineers new to gas treating or with minimal gas treating experience, to develop and maintain the degree of expertise needed to perform at a high level of excellence.

## Contact Us:

Optimized Gas Treating, Inc.

212 Cimarron Park Loop

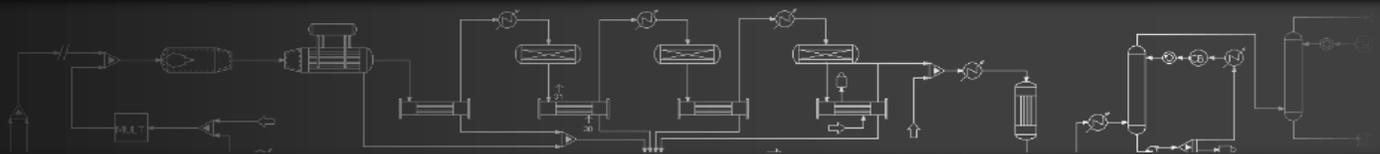
Buda, TX 78610

Phone | Fax +01 512 312 9424

info@ogtrt.com

consulting@ogtrt.com





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[www.ogtrt.com](http://www.ogtrt.com)

**OGT** Inc.  
*Optimized Gas Treating, Inc.*  
212 Cimarron Park Loop  
Buda, TX 78610  
t|f +01 512 312 9424