The CONTACTOR™

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The Origins of ProTreat™

There are three commercially available simulation packages that are either based exclusively on the mass transfer rate approach to tower simulation, or use this approach in one or more modules. They are:

- ***RATEFRAC***®, a module which is part of the SimSci simulation software package Pro-II®,
- ***RateSep***™, (now called Rate-Based Distillation) a RATEFRAC derivative developed by AspenTech and part of the AspenPlus® simulator, and
- ***ProTreat***™, OGT's mass transfer rate based simulator, specifically for gas treating applications using both amines and physical solvents, dehydration, and sour water stripping.

All three simulation tools have their origin in the research carried out from 1965 to 1968 by Optimized Gas Treating's president, Ralph Weiland while a Ph.D. candidate at the University of Toronto(1).

The mass transfer rate approach to CO_2 absorption and solvent regeneration using aqueous *ethylenediamine* was developed by Weiland from the work of Danckwerts and coworkers. The approach was successfully used to correlate and understand the data collected in some two hundred experiments using a continuously-operated 4-inch diameter packed absorber at atmospheric pressure connected to a regenerator of the same size. Some of the details involved in rate-modeling regeneration were fleshed out in further experimental and modeling work on CO_2 stripping from MEA done by Weiland at the University of Queensland, Australia, in the mid-1970s(2).

Serious efforts to develop a mass transfer rate based model for simulating acid gas removal with amines got underway at Clarkson University around 1982 via National Science Foundation funding and through a larger grant to Weiland from the Dow Chemical Company. The work had three components: development of the computer code necessary to run a complete column simulation(3), development of a robust computational method for calculating the speciation (ionic makeup) of gas treating solutions containing multiple† amines(4), and development of experimental data on the fundamental mass transfer coefficients that pertain to contacting on valve-type trays(5). The culmination of this work was the provision to Dow Chemical of a main-frame computer module suitable for the calculation of both absorber and regenerator performance using single- as well as two-amine systems. This model continued to be used and improved by Dow until its GAS/SPEC business was divested to INEOS Oxide as part of Dow's purchase of the assets of Union Carbide Corporation.

In parallel with this work, Dr. Ross Taylor, also at Clarkson University, was doing some fascinating research on the mass transfer rate based simulation of such complex separation processes as azeotropic and extractive distillation, and three-phase distillation. These processes were not amenable to meaningful equilibrium-stage calculation any more than reactive absorption and solvent regeneration were. Mass transfer rate based models were the only ones capable of predicting and explaining some of the strange behaviors, such as negative tray efficiencies, observed in practice.

The work at Clarkson came to the attention of Mr. John van Gelder of Koch Engineering Company Wichita, Kansas. Koch Engineering became involved in three-way negotiations with AspenTech, and the technology's original developers, Professors Taylor & Weiland, with the goal of developing a commercially-viable module for simulating a wide range of columns based on mass transfer rate concepts as the underlying principle. However, the discussions did not proceed to the satisfaction of all the parties. As a result, Taylor and Weiland formed Taylor, Weiland & Associates (TWA) for the purpose of developing a mass transfer rate model for amine treating, and Koch Engineering and AspenTech embarked on the development of RATEFRAC as a general-purpose module for mass transfer rate based distillation.

Dr. M. S. Sivasubramanian (Siva) who, as part

† The potential benefits of using solvents containing two amines were a direct development of work at Clarkson — see Reference 4.

of his Ph.D. thesis under Weiland's supervision at Clarkson, had been responsible for developing a substantial part of the computer code used by Dow Chemical, and who was for a short while employed by TWA, carried the technology and know-how with him when he went to work for AspenTech, specifically to develop their RATEFRAC module. Meanwhile, TWA developed GASPLANT™ and GASPLANT-PLUS™ for single- and mixed-amines, respectively.

It was an unfortunate happenstance that about the time the GASPLANT tool was being completed for use on mainframe computers, personal computers had just started coming onto the market and the Microsoft® Windows® operating system was in its infancy with Windows 3.1. The market for mainframe software vanished almost overnight and there was a scramble to convert GASPLANT into a form suitable for the severely-limited memory available on PCs. In the end, GASPLANT and GASPLANT-PLUS were technical successes but commercial failures. Mass transfer rate based technology in the gas treating arena was much too far ahead of its time and the financial resources necessary to develop a user-friendly PC interface were not available to TWA. All rights to the computer code were sold to ChemShare Corp. which later became WinSim® Inc. In 1998 WinSim merged GASPLANT-PLUS into DESIGN II™ and WinSim continues to offer GASPLANT-PLUS in this form to this day.

In 1992 Optimized Gas Treating was formed by Ralph Weiland (then in Australia) and Jack Dingman for the single purpose of developing a mass transfer rate based simulator for gas treating as a true Windows application. Jack had been an early supporter of the GASPLANT software and believed in the technology enough to spend his retirement years chained to a desk trying to get a new company off the ground. Over the next six years Ralph and two other engineers/programmers in Australia developed the first version of ProTreat from a blank page and had it ready for beta testing commercially by late 1998. The first version was capable of handling a fully flexible flowsheet using up to three of the amines MEA, DGA®, DEA, DIPA and MDEA in a single blend. Over time, other amines such as piperazine as well as all the INEOS GAS/SPEC solvents were added to the software's capabilities. Through extensive use by Mike Sheilan (Amine Experts) and Nate Hatcher (ConocoPhillips) the model's mass transfer parameters were tuned to solidly reliable performance data from dozens of operating amine plants.

Interestingly, Dr. Sivasubramanian joined OGT in early 2003, bringing with him knowledge gained during 15 years at AspenTech as the architect of RATEFRAC. He was involved in adding new capabilities to ProTreat and in hunting out many of the numerous bugs that embed themselves and lurk for amazing periods of time in any software of this magnitude. Siva left OGT at the end of 2008 to pursue other research interests in the bio-fuels area.

Shortly after Siva joined the company, OGT hired its first full-time Sales Engineer, Jaime Nava and from that time forward ProTreat has found itself in rapidly increasing use by consultants, solvent vendors, engineering firms, suppliers of tower internals, and operating companies around the world. Indeed, many of the largest and best known companies now consider ProTreat to be the gas treating simulation standard.

Since the first version became commercial in 2000, OGT has added piperazine (used in the original BASF aMDEA solvent) and AMP, the GAS/SPEC solvents, heat stable salts, stripping promoters such as phosphoric acid. New developments continue to be made including DMPEG (the basic chemical used in SELEXOL solvents), Genosorb, chilled ammonia, cold methanol, and Morphysorb. And with the early 2009 arrival of Nate Hatcher as Vice-President, Technology Development, new capabilities are now being added to ProTreat at a greatly increased pace.

The commercial development of mass transfer rate based column simulation tools has involved remarkably few individuals, all of them closely-connected with each other over many years. The work of the original two developers, Taylor and Weiland, has certainly spawned several highly-valued simulation tools that not only have a common origin but are, and continue to be, tightly interrelated.

(1) Weiland, R. H. and Olev Trass, *Absorption of Carbon Dioxide into Ethylenediamine Solutions*, Parts I & II, Can. J. Chem. Eng., *49*, 767-781 (1971).

(2) Weiland, R. H., M. Y. Rawal and R. G. Rice, *Stripping of Carbon Dioxide from Monoethanolamine Solutions in a Packed Column*, AIChE Journal, *28*, 963-973 (1982).

(3) Sardar, H. and R. H. Weiland, *A Nonequilibrium Stage Approach for the Design and Simulation of Gas Treating Units*, AIChE Annual Meeting, San Francisco, California, November 25-30, 1984.

(4) Chakravarty, T., U. K. Phuklan and R. H. Weiland, *Reaction of Acid Gases with Mixtures of Amines*, Chem. Eng. Prog., p.32, April, 1985.

(5) Scheffe, R. D. and R. H. Weiland, *Mass-Transfer Characteristics of Valve Trays*, I&EC Research, *26*, 228 (1987).