PROCEDE

CAP TECH

A new flowsheeting tool for flue gas treating

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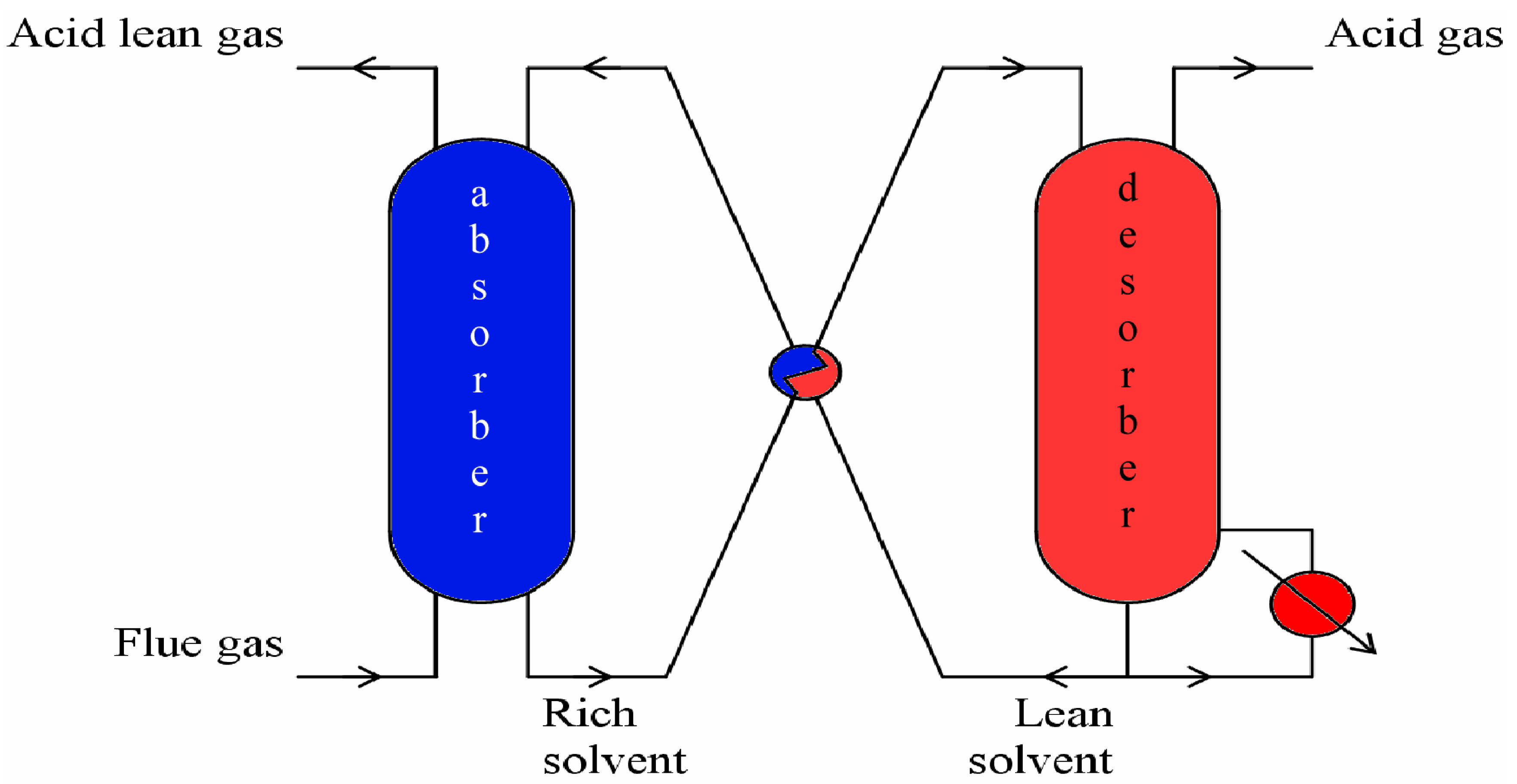
Introduction

A new dedicated acid gas treating process simulator has been developed from scratch. A simplified process scheme is shown below. The simulator however can handle much more complicated systems.



Currently supported thermodynamic models

- **Ideal**
- **Electrolyte Equation of State (E-EOS):**

$$A = A^{IG} + A^{RF} + A^{SR1} + A^{SR2} + A^{LR} + A^{BORN}$$

Helmholtz free energy terms:
Ideal Gas, Repulsive Force, Molecules and Ions Short Range Forces, Long Range Ionic Interaction and Born-term

Typical reactive system (Example: Amine-CO_2-H_2S)

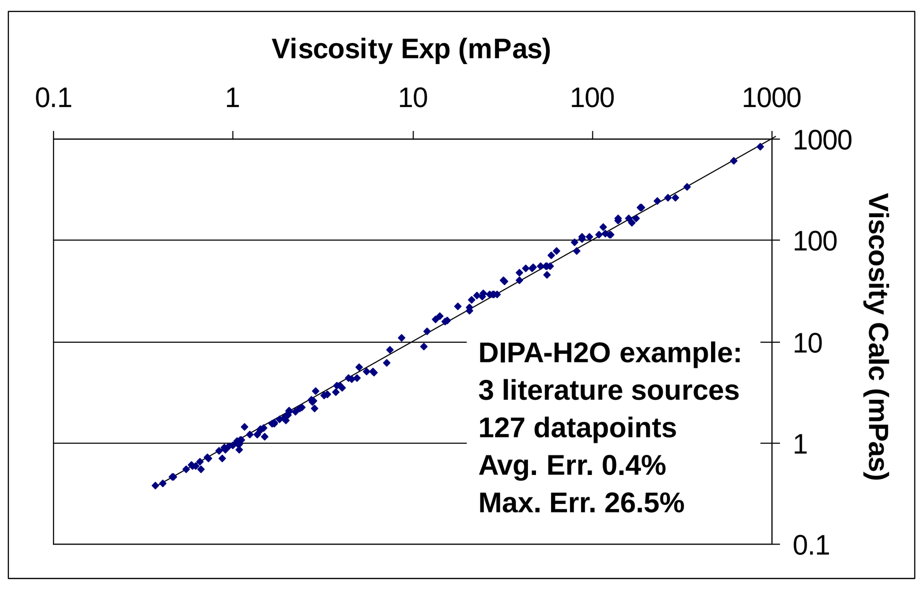
Water dissociation	$2\,H_2O \Leftrightarrow H_3O^+ + OH^-$
Bicarbonate formation	$2\,H_2O + CO_2 \Leftrightarrow H_3O^+ + HCO_3^-$
Carbonate formation	$H_2O + HCO_3^- \Leftrightarrow H_3O^+ + CO_3^=$
H_2S dissociation	$H_2O + H_2S \Leftrightarrow H_3O^+ + HS^-$
Amine protonation	$H_2O + R_3NH^+ \Leftrightarrow H_3O^+ + R_3N$
Carbamate reversion (prim/sec-amine)	$R_3NCOO^- + H_2O \Leftrightarrow R_3N + HCO_3^-$

Major thermodynamic and physical properties

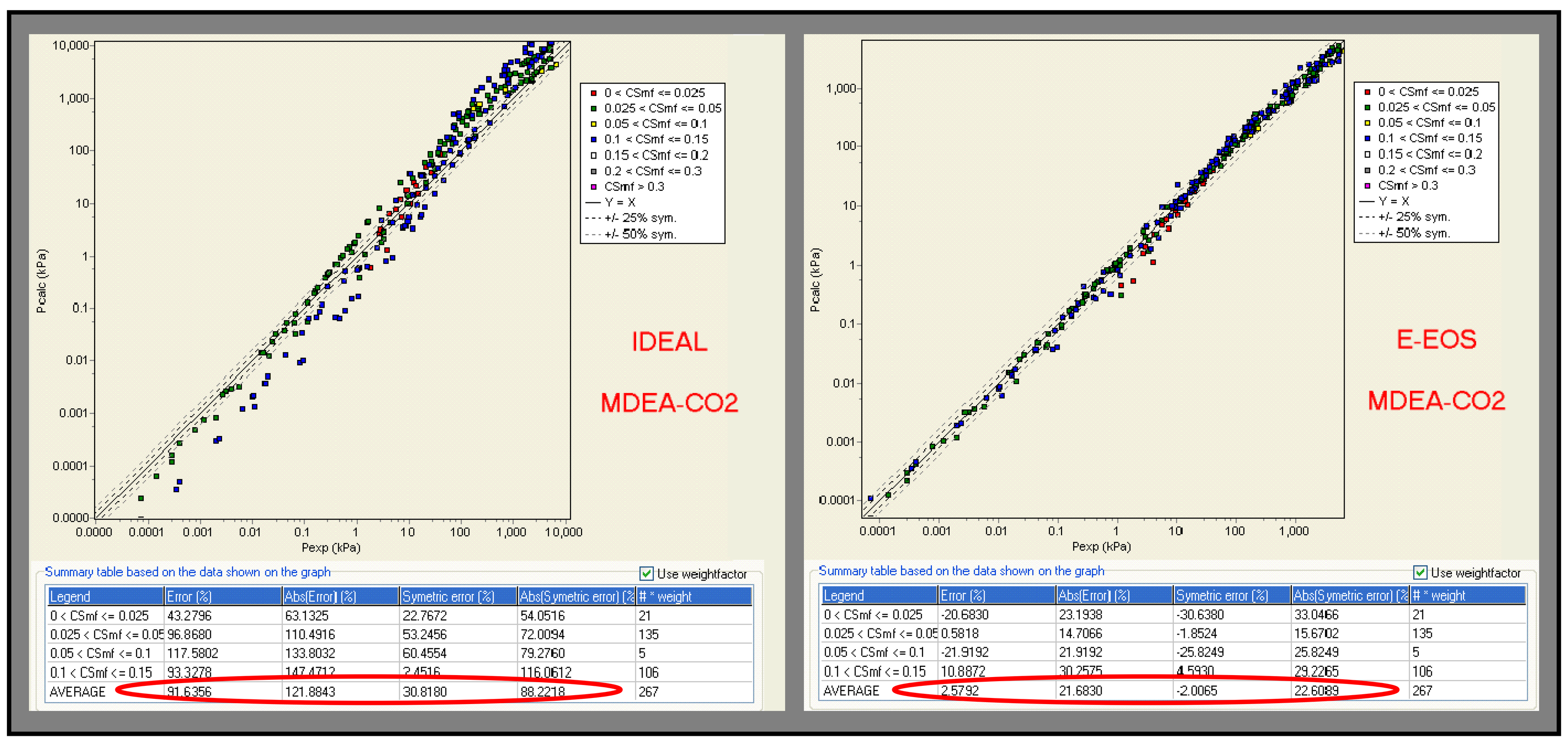
Property	Liquid	Vapor	Mixed
Enthalpy	Yes	Yes	Yes
Heat capacity	Yes	Yes	Yes
Density	Yes	Yes	Yes
Viscosity	**Yes**	Yes	No
Thermal conductivity	Yes	Yes	No
Surface tension	Yes	No	No

New liquid viscosity model →

(required for accurate rate-based modeling)



VLE-results MDEA-CO_2 (Ideal vs E-EOS)



Equilibrium-based unit operations

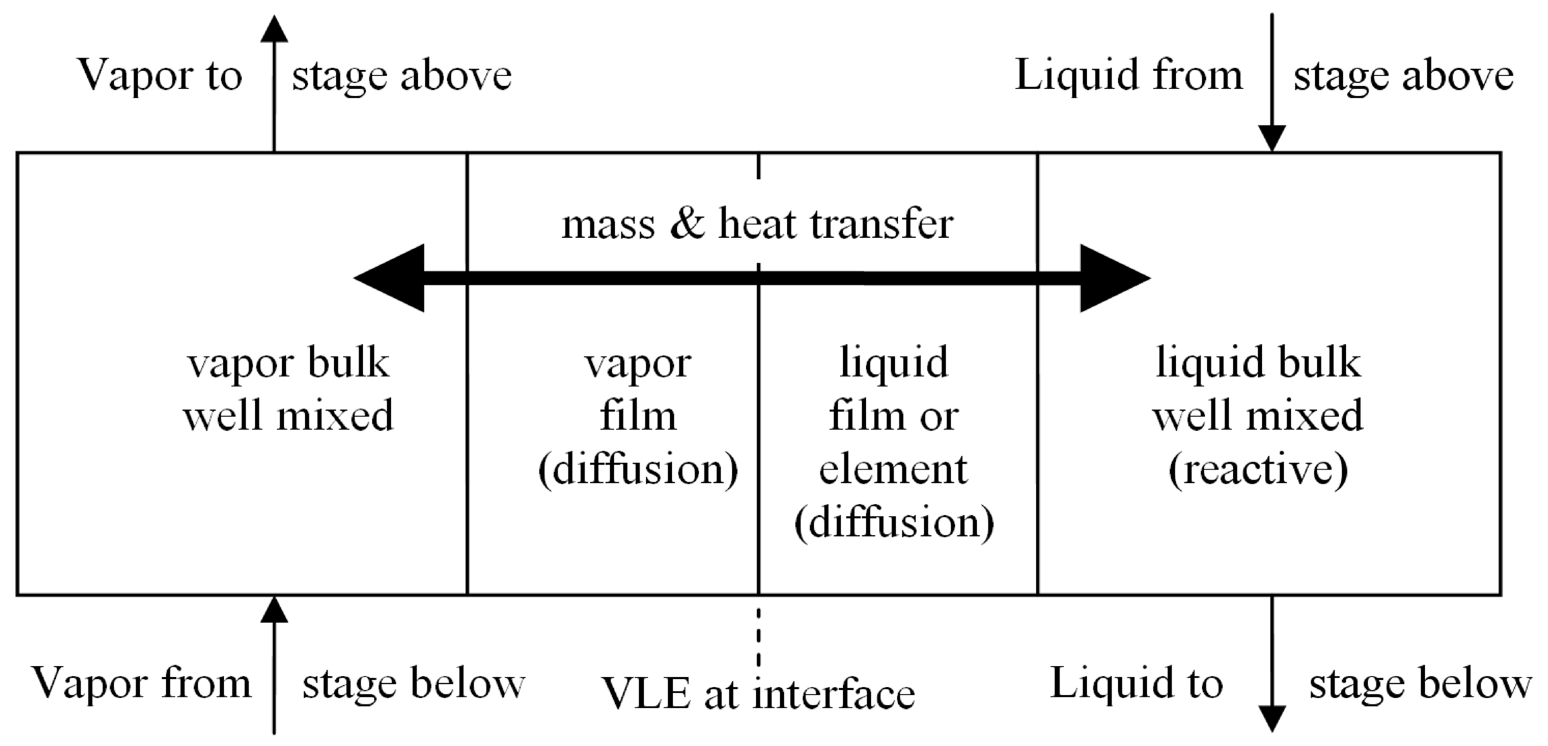
Separation	Separator, Flash drum, Column
Heat exchangers	Heater/cooler, Heat exchanger
Pressure changers	Pump, Turbine, Compressor, Expander, Appendage
Flowsheeting	Inlet, Outlet, Recycle, Mixer, Splitter
Gas treating	Formulator, Thermodynamic model fitting

Rachford-Rice:

$$\sum_i \frac{z_i(1-K_i)}{1+V(K_i-1)} = 0$$

$$K_i = \frac{y_i}{x_i}$$

Rate-based unit-operations: Columns



Column models (continued)

Hydrodynamic models (pressure drop & flooding)

Trays	Dumped packing	Structured packing
Perry	Leva 1992	Bravo 1986 Bravo 1992

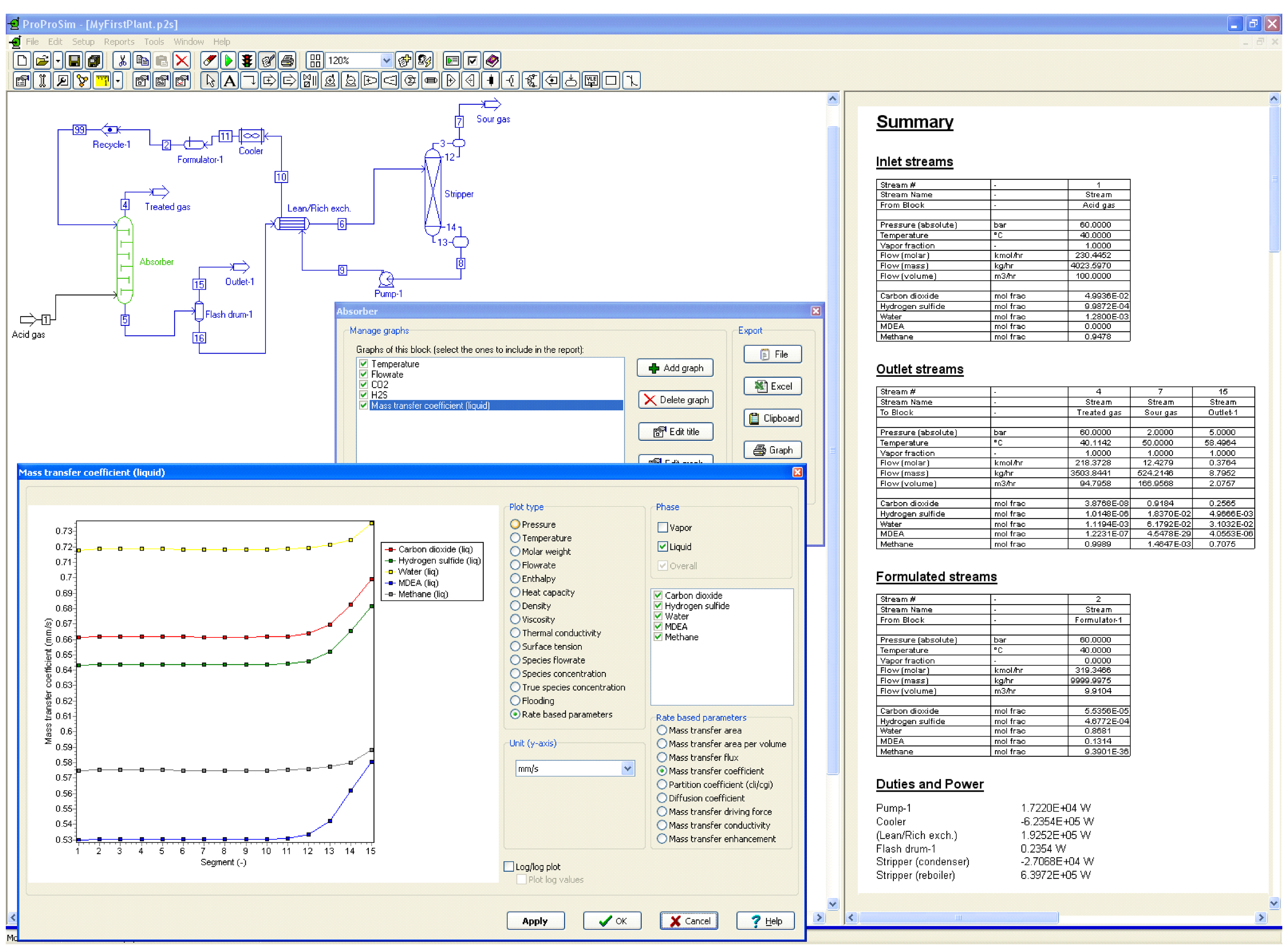
Mass transfer models (k_g, k_l, area)

Trays	Dumped packing	Structured packing
Zuiderweg 1982 Bennet 1993 Scheffe 1987 AIChE 1958 Chan 1984	Onda 1968 Bravo 1982 Billet 1992	Bravo 1985 Bravo 1992 Shetty 1997 Olujic (Delft model) 2002 Onda 1968 Billet 1992

Other models

- **Heat transfer coefficients: Chilton-Colburn analogy**
- **Vapor diffusion coefficients: Fuller / Blanc**
- **Liquid diffusion coefficients: Wilke-Chang / Versteeg**
- **Chemical enhancement of mass transfer:**
  - **Higbie penetration model (Rigorous numerical solution)**
  - **Wellek (Approximate analytical solution)**

Screenshot



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More information can be found on www.co2-captech.nl.