Life Cycle Economic Optimization As Opposed to Design Heuristics
Natural Gas Dryers As An Example

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Problem Motivation

- **Global Zeolite Market**
  - Continual growth over the years
  - Total Market Value of $3.5 billion as of 2014[1]
  - Zeolites are used primarily as adsorbents or catalysts

http://qwtjlive.com

- **Swing Adsorption Process**
  - Adsorption Processes are used for a variety of applications
  - Typical design approach relies on assumed parameters
  - Example: Natural gas dehydration (Manning & Thompson, 1990)
  - Optimal Design is not guaranteed.

- **Importance of Optimal Design**
  - Market size is expected to increase
  - Deficiencies in conventional design approaches.

(1) http://en.wikipedia.org/wiki/World_energy_consumption
(3) http://globalchange.mit.edu/files/document/MITJPSPGC_Rpt271.pdf

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Design Approaches

Common approach used based upon experimentally determined "effective" sorbent capacity in mol/kg & Target Pressure Drop (Wunder, Oil & Gas, 1962)

Rely on assumed cycle timings and simplified model of the cycle

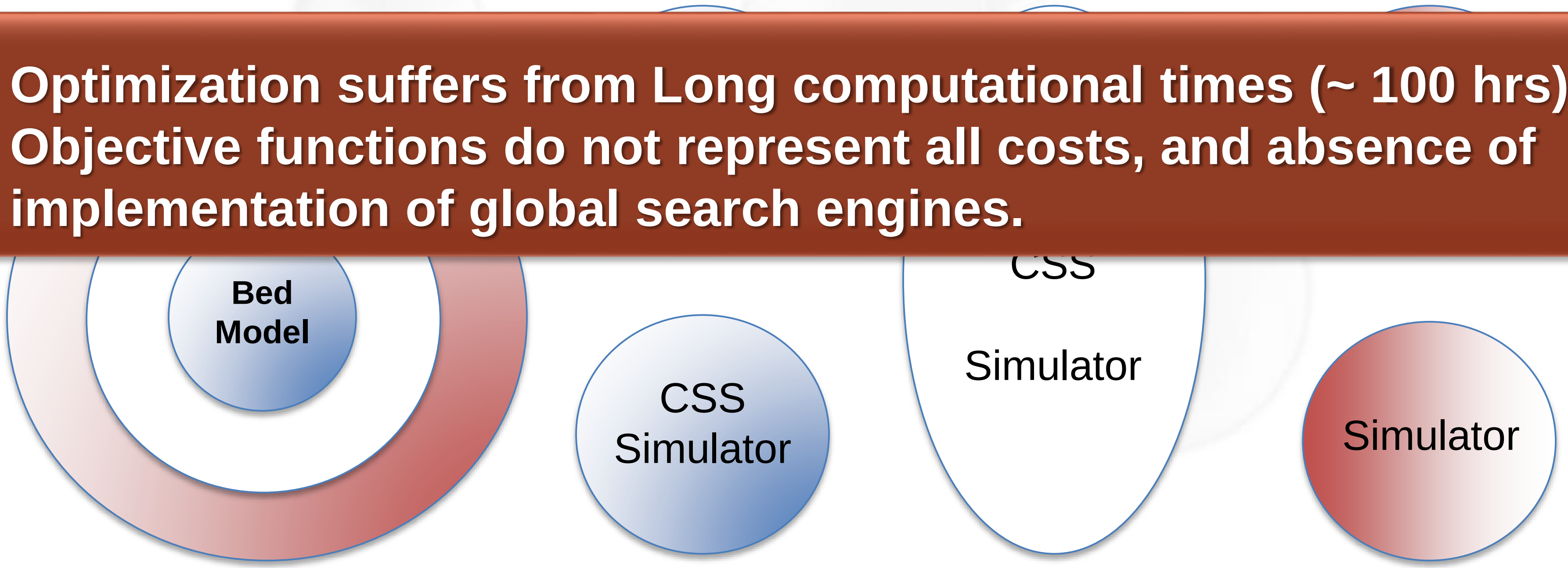
We Target An Optimization Design Protocol which Assures design optimality by Virtue of Lowest NPV while capturing the complexities of kinetics

Net Present Value of total costs during project life (NPV) is not considered

Design can satisfy the requirement but no knowledge on possible cost savings

- **General Comments:**
  - Literature Focuses on PSA.
  - Optimization Coupled with Kinetics and tackled simultaneously.
  - Most of studies focus on single point optimization.
  - Objective functions considered do not represent all costs

Optimization suffers from Long computational times (~ 100 hrs), Objective functions do not represent all costs, and absence of implementation of global search engines.



(a) (Jiang et al. ,2003) (Sankararao et al., 2007) (Jiang et al. ,2003)

CSS: Cyclic Steady State

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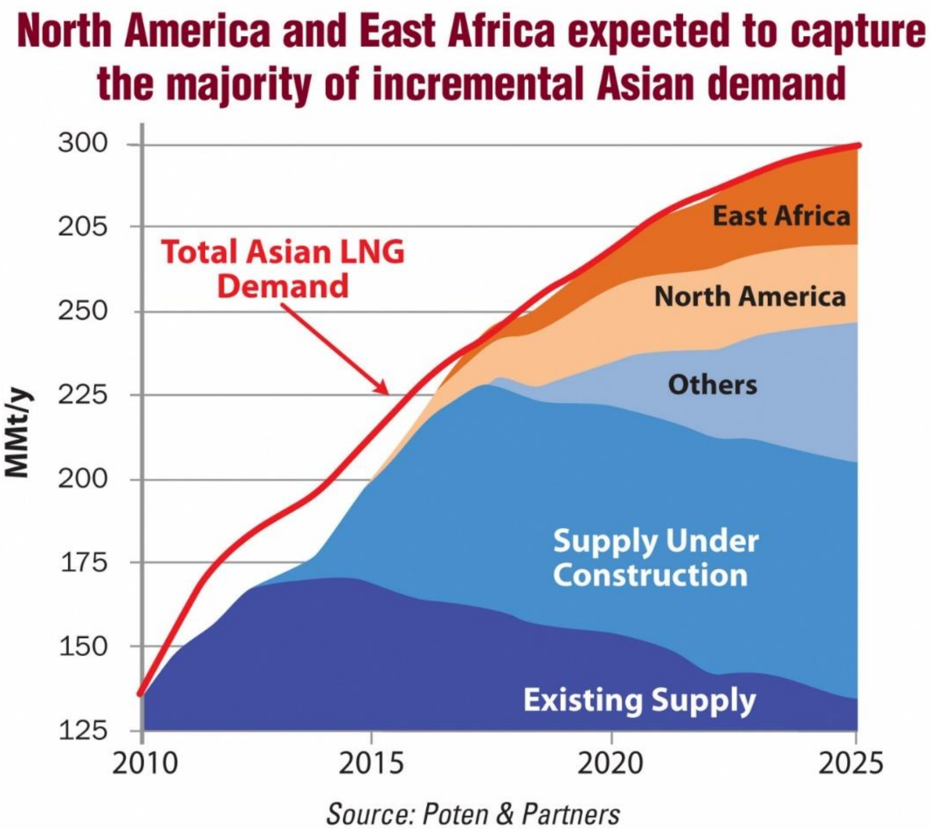
Case Study – Natural Gas Drying

- **World LNG Demand:**
  - LNG Market is Expected to Increase in the coming future
- **Dehydration of Gas:**
  - Natural Gas used for LNG is dehydrated by Molecular Sieves.
  - Total Market Size of LNG ranges between 120 to 160 billion as of 2014(3)
- **Importance of Optimal Design**
  - Market size and expected increase LNG demand.
  - Substantial savings expected.



http://www.alaskajournal.com/business-and-finance/2013-12-04/lng-101-spot-market-pricing-economics

(1) http://en.wikipedia.org/wiki/World_energy_consumption
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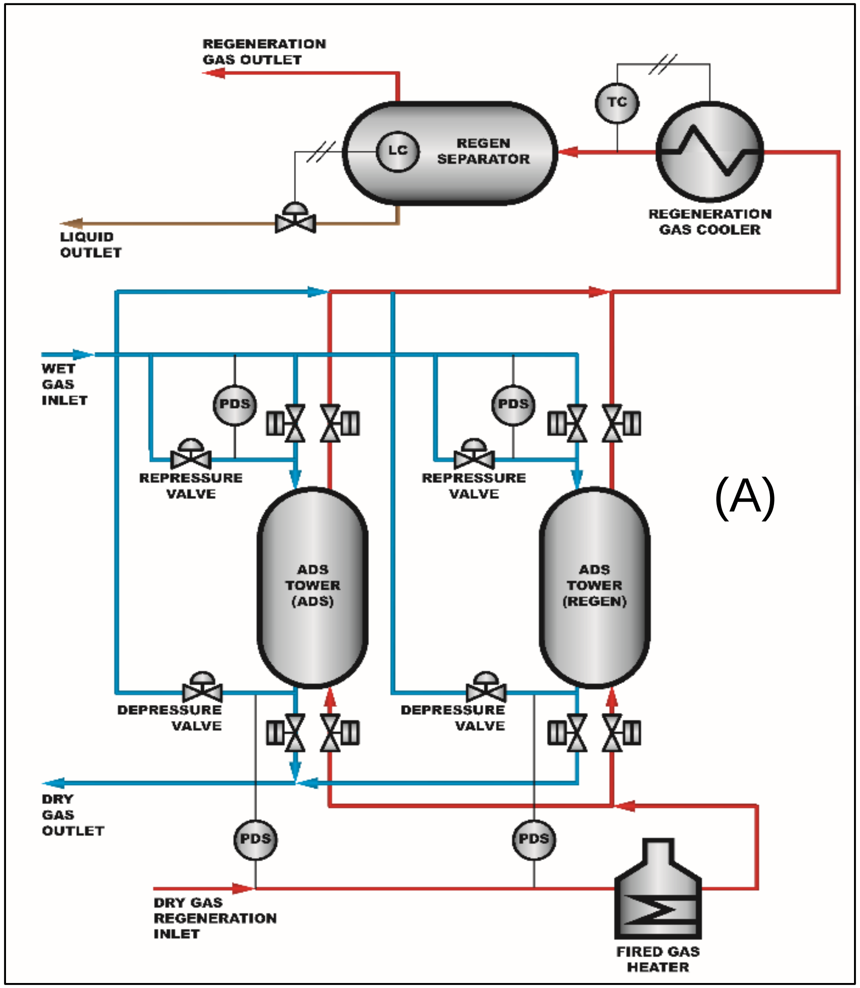
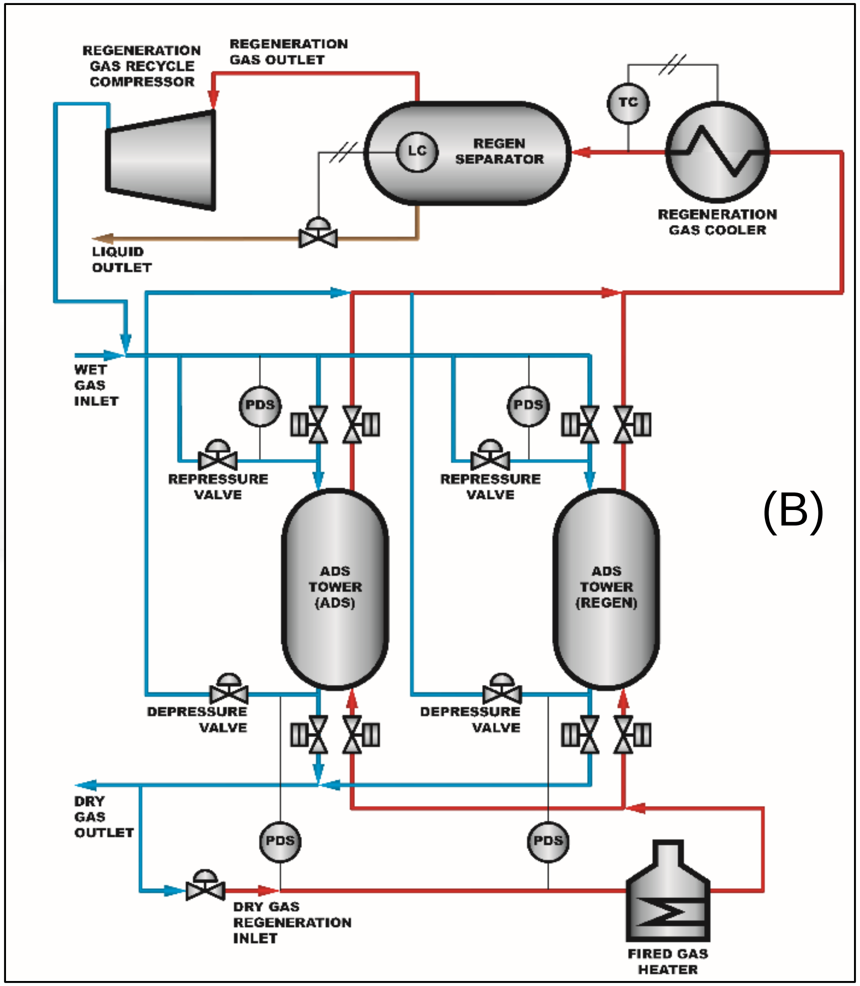
Typical Process Schemes for NG Dehydration



(A)



(B)

F. S. Manning and R. E. Thompson, *Oilfield Processing of Petroleum: Natural gas*: PennWell Books, 1991.

The Optimization Problem Structure

- Objective function is the Net Present Value of Costs (NPVC).
  - Composed of three elements: Total Capital Investment, OPEX, and Bed Replacement.
- Eight design variables.
- Four Constraints.

Objective Function Challenge

$$NPVC = \underbrace{6\cdot\left(P_{bed}+P_{v}+P_{FHR}+P_{comp}+P_{HxC}+P_{Sep}\right)}_{TCI}+$$
$$\underbrace{\sum_{j=1}^{J}\left(P_{W}+P_{HDR}+P_{CW}\right)\left(\frac{1+r_{\inf}}{1+r_{dis}}\right)^{j}}_{OPEX}+\underbrace{\sum_{j=n^{*}f}^{J}\left(P_{bed}\right)\left(\frac{1+r_{\inf}}{1+r_{dis}}\right)^{j}}_{BED}$$

Constraint Description	Kinetic Model Challenge
Assigned adsorption cycle time should not exceed the breakthrough time predicted via simulation given L,D and N.	$t_{ads} \le t_{ads,\max}$ (2)
Total regeneration time should not exceed the assigned adsorption cycle time.	$t_{ads} \ge \frac{N_{ads}}{N_{reg}}\left(t_{reg}+t_{heating}+t_{cooling}\right)$ (3)
Assigned regeneration cycle should exceed the minimum required time for regeneration predicted via simulations given L,D, N and N_1	$t_{reg} \ge t_{reg\min}$ (4)
TSA unit pressure drop should not exceed the maximum allowable pressure drop ΔP_{max}	$\Delta_{\max} \ge L\left(\frac{150\mu(1-\varepsilon_b)^2 U_f}{4R_p^{2}\varepsilon_b^{3}}+\frac{1.75\rho_f(1-\varepsilon_b)U_f^{2}}{2R_p\varepsilon_b^{3}}\right)$ (5)

Design Variable	Description
L	Bed Length (m)
D	Bed Diameter (m)
N_{ads}	Number of Vessels undergoing adsorp.
N_{reg}	Number of Vessels undergoing regen.
Q_{reg}	Molar flow of regeneration gas (kmol·h^{-1})
T_{regG}	Temperature of regeneration gas (ºC)
t_{reg}	Allocated time for regeneration (h)
t_{ads}	Adsorption cycle time (h)

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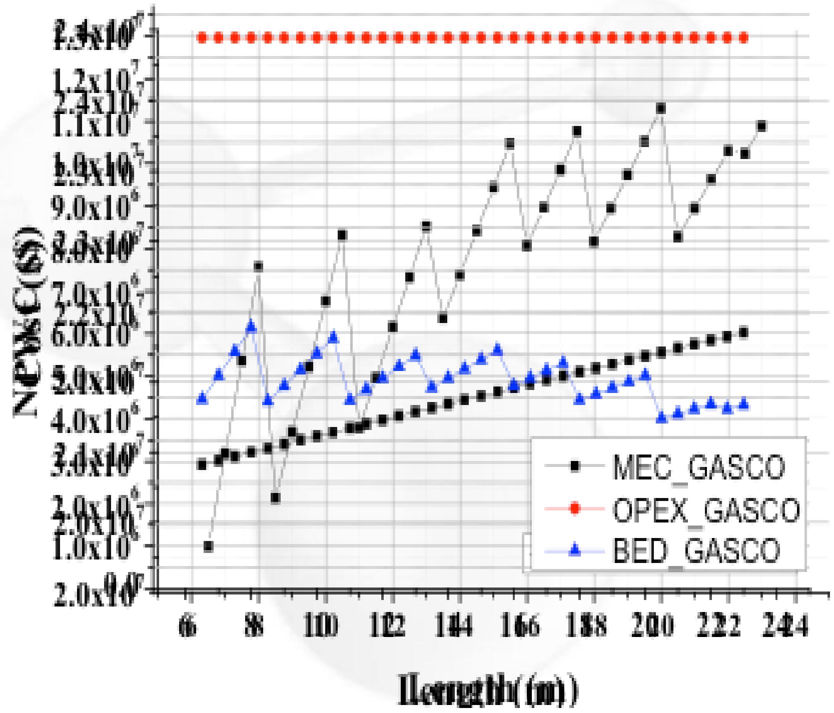
Addressing Objective Function Discontinuities

Source of discontinuities is Bed Replacement.

Discontinuities occur at ordered periods.

Minimum cost occurs at the beginning of the period



Addressing Objective Function Discontinuities

Break the space of NPVC into continuous segments by using period f as an integer variable

$$f = \mathrm{int}\left(\frac{t_{ads} \cdot N_R}{4380}\right)$$

The Kinetic Model

- Utilize the equilibrium solution of Rhee and Amundson (Rhee et al, 1973) corrected for mass transfer effects with a factor.
- Cycle simulate phase change (Wunder et al, 1962)

$$\frac{\partial C_i}{\partial t} + \frac{\partial (uC_i)}{\partial z} + \frac{1-\varepsilon_b}{\varepsilon_b}\frac{\partial q_i}{\partial t} = D_{z,i}\frac{\partial^2 C_i}{\partial z^2}$$

$$\frac{\partial q_i}{\partial t} = k_{mass,i}\left(q_i^* - q_i\right)$$

$$\frac{\partial T}{\partial t} + \frac{\partial (uT)}{\partial z} + h_b \frac{a_{b/P}}{C_b \rho_f}\left(\frac{1-\varepsilon_b}{\varepsilon_b}\right)\left(T - T^P\right) + \frac{4h_b}{D\varepsilon_b C_b \rho_f}\left(T - T_s\right) = 0$$

$$\frac{\partial T_P}{\partial t} = h_s \frac{a_{b/P}}{C_P \rho_P}\left(T - T_P\right) - \frac{1}{\rho_P C_P}\sum_{i=1}^{Nu} H_{ads,i}\frac{\partial q_i}{\partial t}$$

$$\frac{\partial T_s}{\partial t} = h_b \frac{a_{b/P}}{C_{P,v}\rho_v}\left(T - T_s\right)$$

$$-\frac{\partial P}{\partial z} = \frac{150\mu\left(1-\varepsilon_b\right)^2 u}{4R_P^{\,2}\varepsilon_b^{\,3}} + \frac{1.75\rho_f\left(1-\varepsilon_b\right)u^2}{2R_P\varepsilon_b^{\,3}}$$

$$C_i\left(t=0, z \neq z_B\right) = C_{i,ini} \qquad C_i\left(t, z = z_B\right) = C_{i,o}$$

$$uC_i\left(t, z = z_B\right) = uC_i^o - D_{z,i}\left.\frac{\partial C_i}{\partial z}\right|_{z=z_B}$$

$$T\left(t, z = z_B\right) = T_o \qquad T(t=0, z) = T_{ini}$$

$$k_{mass,i} = \left(\frac{q_i^*}{y_i k_{fi}\rho_f a_{b/P}} + \frac{R_P}{5a_{b/P}}\left(\frac{1}{D_{P,i}} + \frac{\tau}{\varepsilon_P D_{m,i}}\right)\right)^{-1}$$

$$C_i = \frac{y_i P}{RT}$$

$$k_{m,b,i} = \frac{0.357}{\varepsilon_b}\mathrm{Re}^{0.64} Sc_i^{033}\frac{D_{m,i}}{2R_P} \qquad h_b = \frac{0.357}{\varepsilon_b}\mathrm{Re}^{0.64}\mathrm{Pr}^{033}\frac{k_{H,g}}{2R_P}$$

$$q_i^* = \frac{K_i \exp\left(\frac{H_{ads,i}}{R}\left(\frac{1}{T_P} - \frac{1}{T_{ref}}\right)\right) q_i^{sat} C_i}{1 + \sum_{i=1}^{Nu} K_i \exp\left(\frac{H_{ads,i}}{R}\left(\frac{1}{T_P} - \frac{1}{T_{ref}}\right)\right) C_i}$$

$$t_{ads} \le \frac{\zeta_{ads} L}{\left(U_f / \varepsilon_b\right)}\left(1 + \frac{1-\varepsilon_b}{\varepsilon_b}\rho_C \frac{\min\left(K_{i,ads}\cdot q_{si}\right)}{1 + \sum_{i=1}^{n} K_i C_i^F}\right)$$

$$t_{reg} \ge \frac{L}{\zeta_{reg}\left(U_{reg}/\varepsilon_b\right)}\left(1 + \frac{1-\varepsilon_b}{\varepsilon_b}\rho_C \max\left(K_{i,reg}\cdot q_{si}\right)\right)$$

$$\zeta = f(\mathrm{Re}, Pe, \ldots)$$

Optimization

Need to assure local optimality and provide confidence on the globality of the optimal solution.

Employ a random initial guess generator while doing optimization for 100 initial guesses.

How to address the MINLP?

Resolve the MINLP to NLPs for every possible combination of integer variables values.

Overall Algorithm for Optimization[1]

- **Optimization Step 1**
  - Use Rhee et al. solution for the isothermal equilibrium adsorption/regeneration case[2].
  - Use of efficiency factors might cause deviations from reality.
  - Algorithm assumes phase change like regeneration
  - Algorithm do not include temperature temporal and spatial variations.
  - Account for vessel steel heating.

- **Optimization Step 2**
  - Use solution of Step 1 as initial guess
  - Full Cycle Optimization Done using Gproms 4.0
  - Solve governing mass and energy PDEs.
  - Losses to vessel steel included in the model.

(1) Al Wahedi et al., CES, 2015
(2) (Rhee et al., Trans. Of Roy. Soc. Of London, 1972)

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Implementing the Algorithm

Assumptions:

- 20-100 kPA Pressure drop
- Pellet Dia. is 1 cm
- 1000 regenerations
- Adsorbent cost 1.7 $/kg

Category	Feed Gas
Pressure (bar)	69.3
Temperature (°C)	28
Compressibility Factor	0.82
Feed Flow (kmol h^{-1})	31,525
Methane	0.831
Ethane	0.0873
Propane	0.0422
i-Butane	0.00831
n-Butane	0.0157
i-Pentane	0.00427
n-Pentane	0.00393
n-Hexane	0.0032
Nitrogen	0.00319
H_2O	0.00071

Adsorbent:

- Zeolite 3A(1)
- Design Capacity at end of life.
- Void fraction of 0.4

(1) M. Simo et al, Ind Eng Chem Res, 2009

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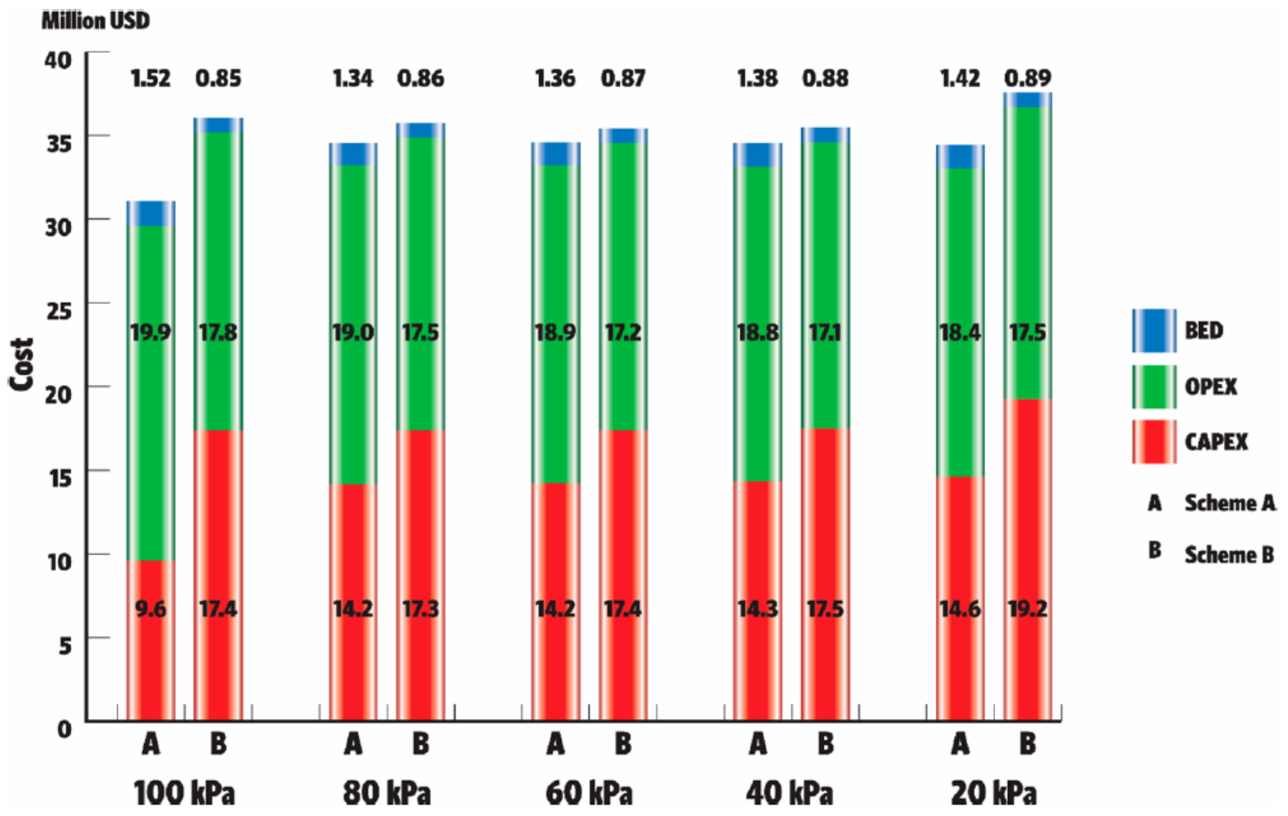
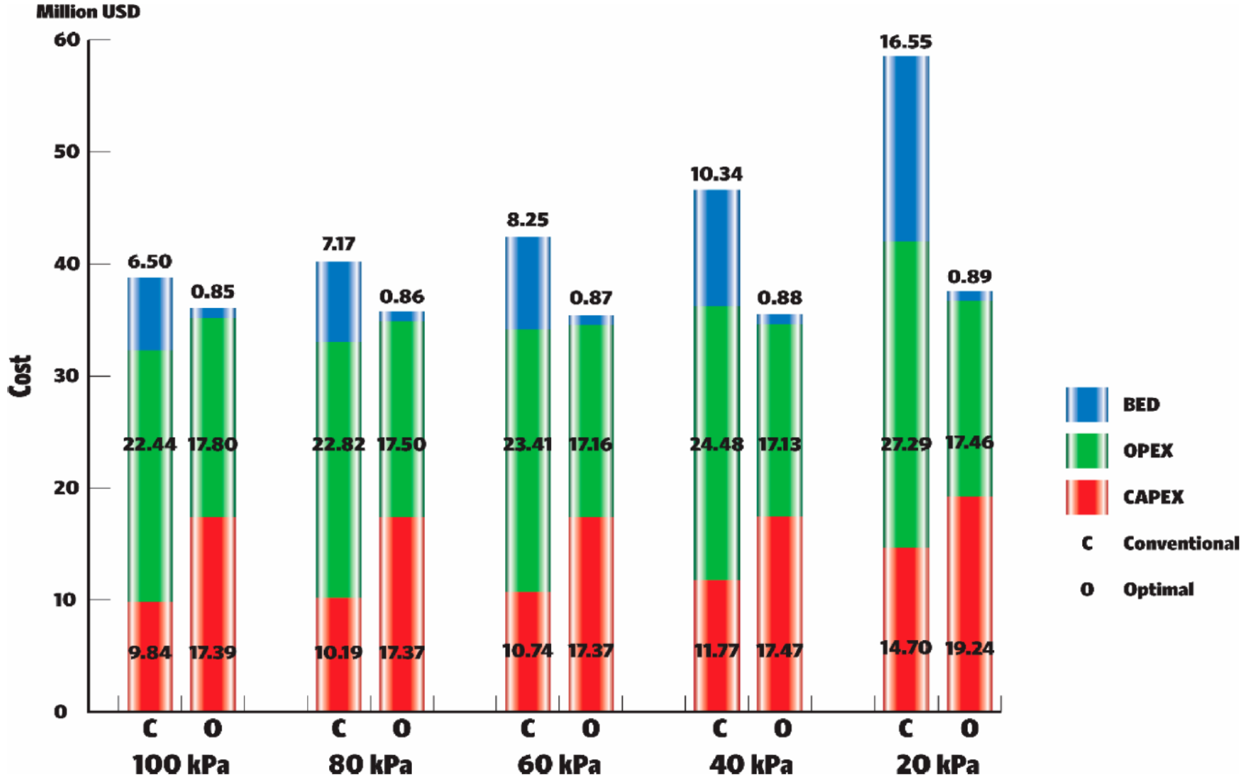
Case Study 1 Scheme A vs. Scheme B

- Total computational time is ~2 hours per case
- OPEX comprise the majority of the cost



Case Study 2 Conventional Design vs. Optimal

- **Conventional as per Thompson and Manning (Thompson & Manning, 1990)**
- **Optimal approach leads to substantial savings (~30%) at lower pressure drops**
- **Caused by substantial reduction in OPEX & BED at the expense of CAPEX (TCI)**



Conclusions

- **Opportunity for optimizing long term cost in dehydration processes' design.**

- **Operating Costs (OPEX) comprises the majority of the NPV and hence must be considered over the course of the plant life.**

- **For the studied case, computed NPV ranged from 4.3 to 5.1 $/MMSCF while OPEX ranged from 2.1 to 2.9 $/MMSCF.**

- **The importance of considering NPV as the objective function.**

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