Optimal Shale Gas Flowback Water Desalination under Correlated Data Uncertainty

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Motivation

Introduction

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- Shale gas hydraulic fracturing demands large amounts of water, on average **9000-29000** m3 of water to complete each well (*Yang el al. 2014*). (10% used in drilling and 90% in hydraulic fracturing).
- A fraction of the water used for drilling and hydraulic fracture **return to the surface** (between 10% and 70%) with typical values around 35%.
- Consequently, high volumes of wastewater from shale gas well pads are generated. As an example, a production forecast for the Marcellus play suggests that **Pennsylvania** will generate **over half billion cubic feet per year by 2025** (*Gay et al. 2012*)
- Most of the water returns to the surface in the first two weeks -**flowback** water- then it tends to stabilize and continues producing water during the whole life of the well -**produced** water-.
- The flowback water include part of the additives included in the hydraulic fracturing fluid: Proppant (sand); Friction reducers; surfactants, scale inhibitors, Biocide, etc. And other compounds depending on the geological characteristics of the shale.

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Motivation

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Typical range of concentrations for some common constituents of flowback/produced water from natural gas development in the Marcellus shale.

(Data compiled by Elise Barbot, University of Pittsburgh, and Juan Peng, Carnegie Mellon University.)

Constituent	Low (mg/l)	Medium (mg/l)	High (mg/l)
Total dissolved solids	66000	150000	261000
Total suspended solids	27	380	3200
Hardness (as $CaCO_3$)	9100	29000	55000
Alkalinity (as $CaCO_3$)	200	200	1100
Chloride	32000	76000	148000
Sulfate	Not Detected	7	500
Sodium	18000	33000	44000
Calcium, total	3000	9800	31000
Strontium, total	1400	2100	6800
Barium, total	2300	3300	4700
Bromide	720	1200	1600
Iron, total	25	48	55
Manganese, total	3	7	7
Oil and grease	10	18	260
Total radioactivity	Not Detected	Not Detected	Not Detected

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Motivation

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Salinity of the flowback waters from various shales expressed in terms of Total Dissolved Solids (TDS).

Shale	Average TDS, ppm	Maximum TDS, ppm
Fayetteville	13,000	20,000
Wooford	30,000	40,000
Barnett	80,000	> 150,000
Marcellus	120,000	> 280,000
Haynesville	110,000	> 200,000
Lebien	~ 16,000 - 70,000 *	
Lubocino	~ 17,000*	

** Estimated by correlation with other parameters.*

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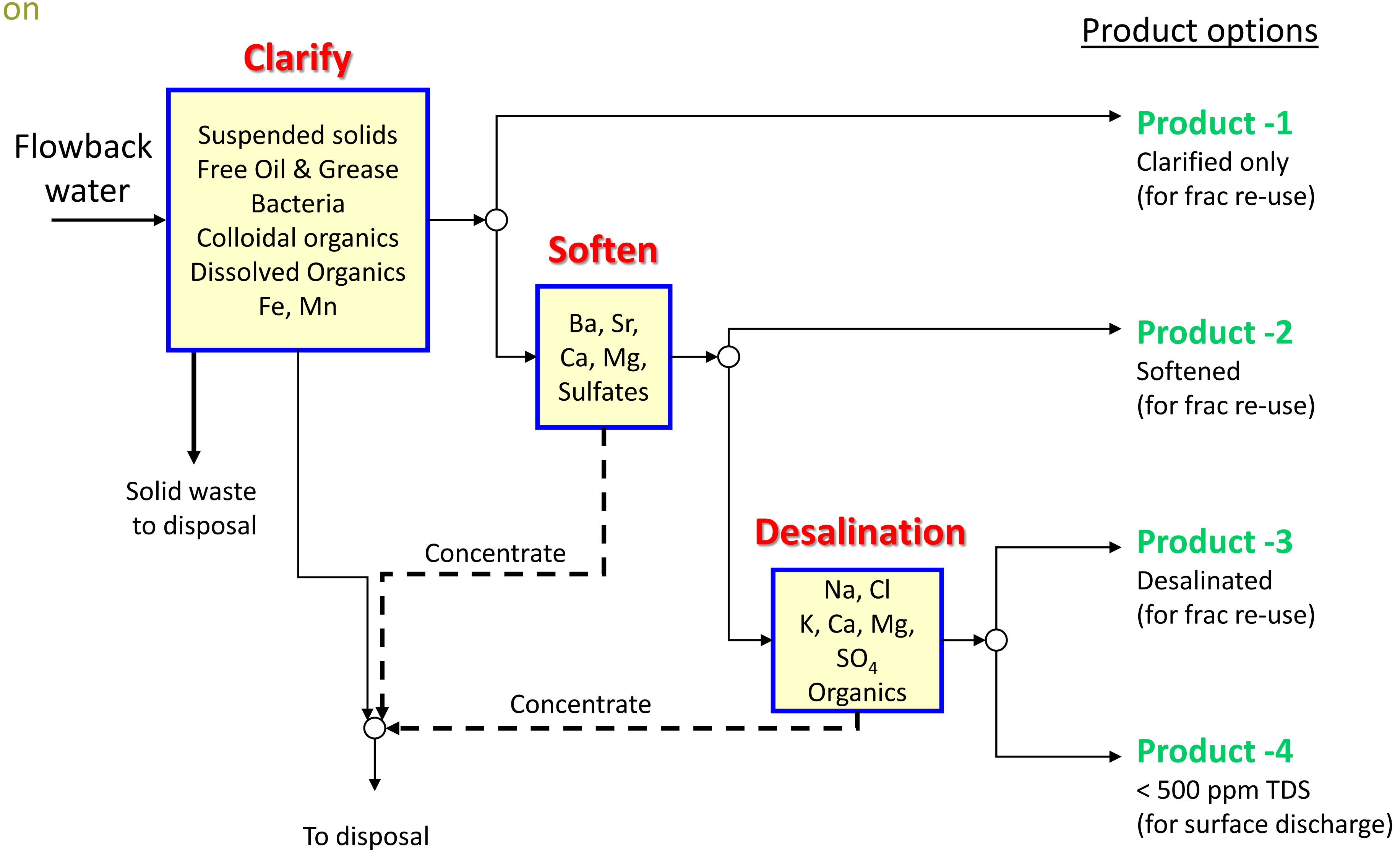

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Motivation

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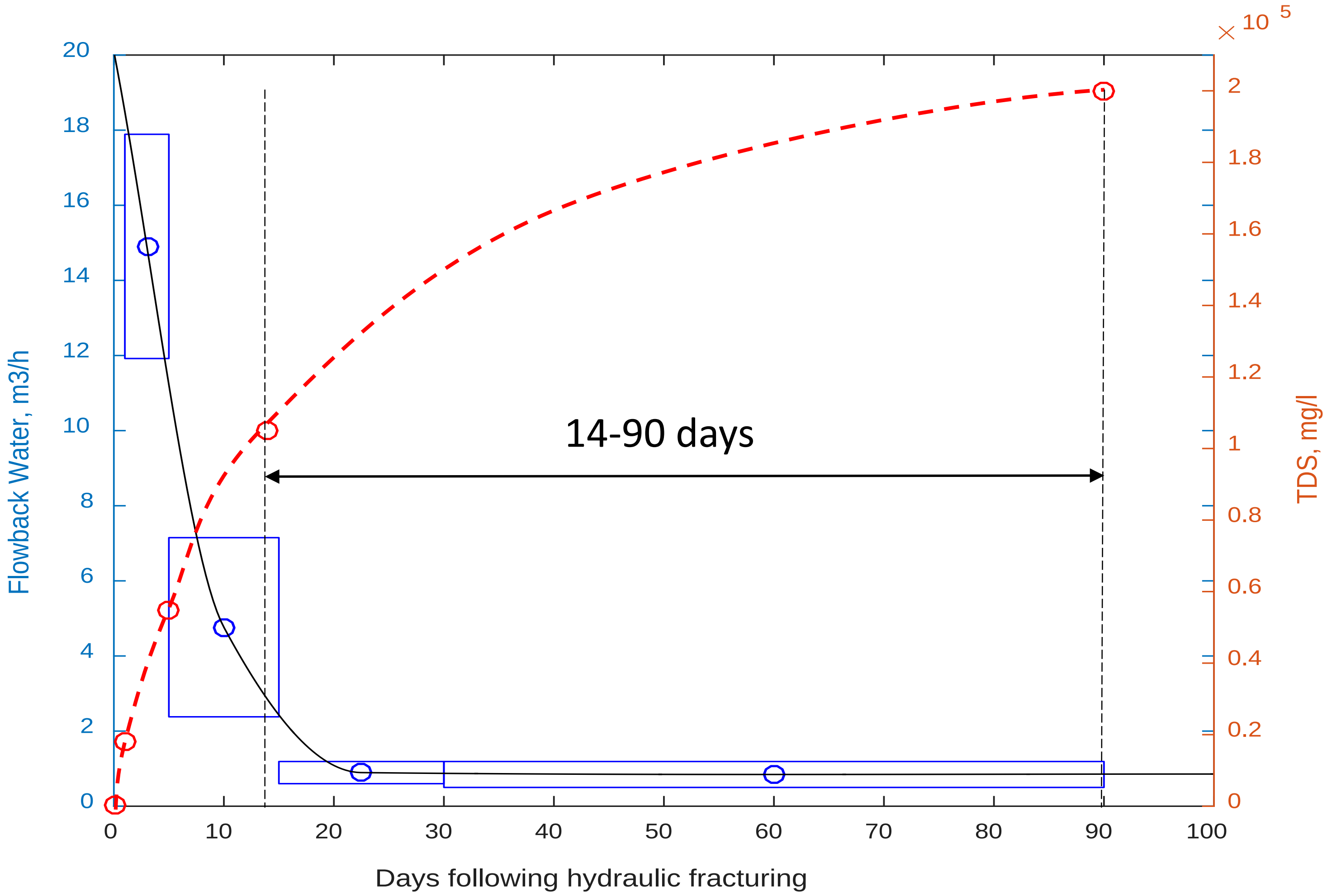

Challenges, design for:

Large water flow and medium salinity

vs.

Low water flow and very high salinity

Uncertainty on both:

Water flowrate and concentration

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Motivation

Introduction

- To address these issues, we introduce **a two stage stochastic model** for the robust design of ZLD desalination systems under uncertainty
- In this new approach, **wastewater salinity and flowrate are both treated as uncertain design parameters**: The uncertainty is mainly related to the great variability presented in well data from real shale plays
- To the best of our knowledge, this is the first study assessing the impacts of data uncertainty on the optimal design **of ZLD evaporation systems**, specially developed for high-salinity shale gas wastewater
- Also, important improvements on the **MEE-MVC** process are implemented, including the use of an external energy source to avoid oversized equipment and the consideration of variable compressor efficiency that allows obtaining a more precise and robust operating performance

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Problem statement

ZLD desalination under uncertainty

- Given is a high-salinity stream of shale gas wastewater, with known inlet state (described by temperature, and mean values for salt concentration and flowrate) and target condition defined by the ZLD specification
- Furthermore, desalination system and energy services (steam and electricity) are also provided with their corresponding costs
- Salt concentration and flowrate of the inlet water stream are both considered as uncertain design parameters that can be explicitly expressed through a set of correlated feeding scenarios with given probability of occurrence

The new stochastic modelling approach is aimed at obtaining a robust design of MEE-MVC desalination systems by reducing brine discharges and energy consumption, while accounting for different feeding scenarios. The MEE-MVC system should be able to efficiently operate at ZLD condition in a large range of correlated feeding scenarios

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Process description

Superstructure

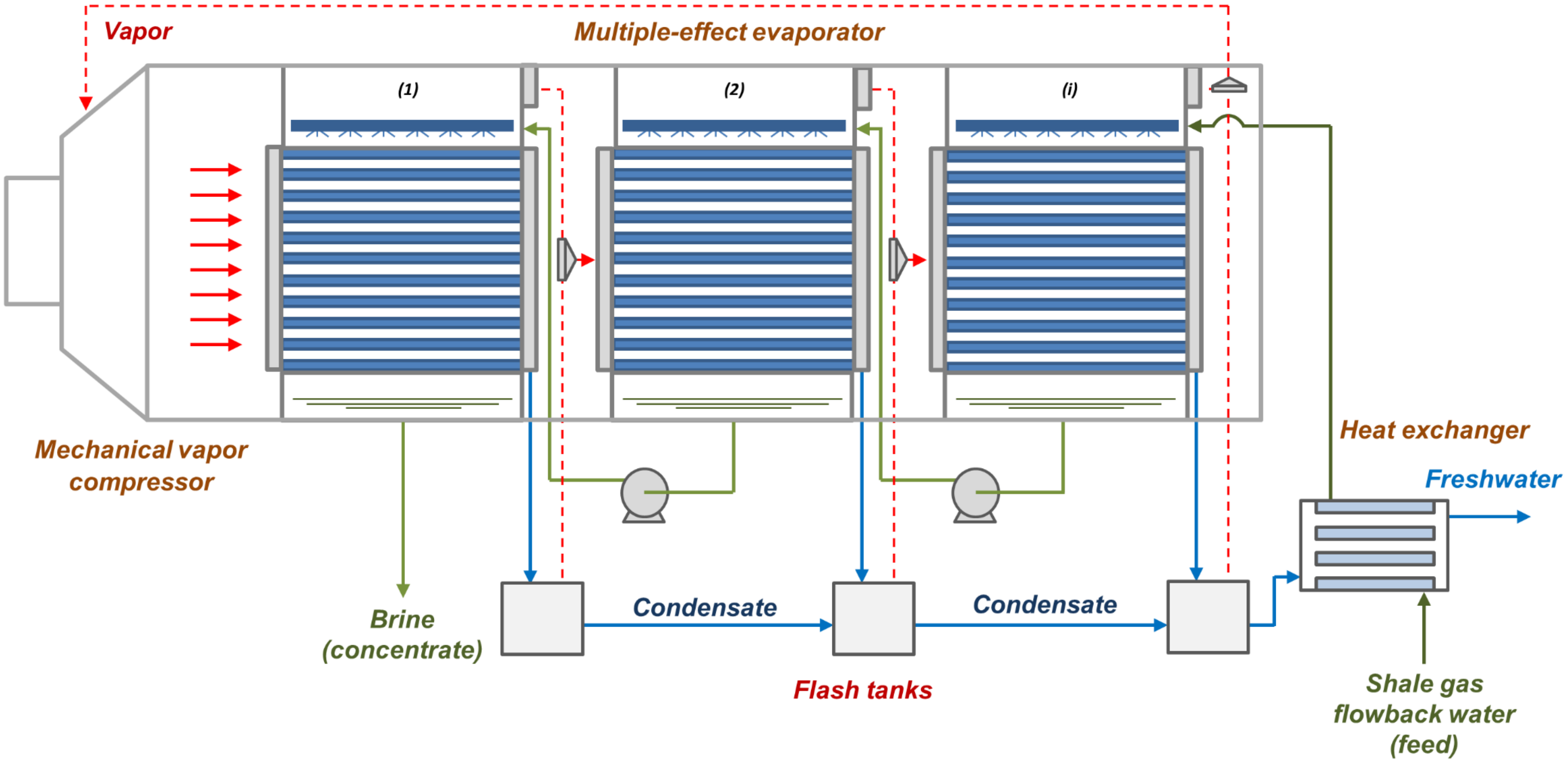

Figure 1. General superstructure proposed for the MEE-MVR desalination plant of wastewater from shale gas production

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Two stage stochastic model

Mathematical modelling approach

- Sizing equations for all equipment
- Mass and energy balances
- Temperature and pressure feasibilities
- Design constraints (ZLD operation)
- Objective function

Index sets

$$I = \{ i \,/\, i = 1, 2, \ldots, I \ \text{ is an evaporation effect} \}$$

$$S = \{ s \,/\, s = 1, 2, \ldots, S \ \text{ is a feeding scenario} \}$$

Decision variables

- **First stage (here and now): sizing-related variables (*e.g.*, volumes, and heat transfer areas)**
- **Second stage (wait and see): all remaining optimization variables**

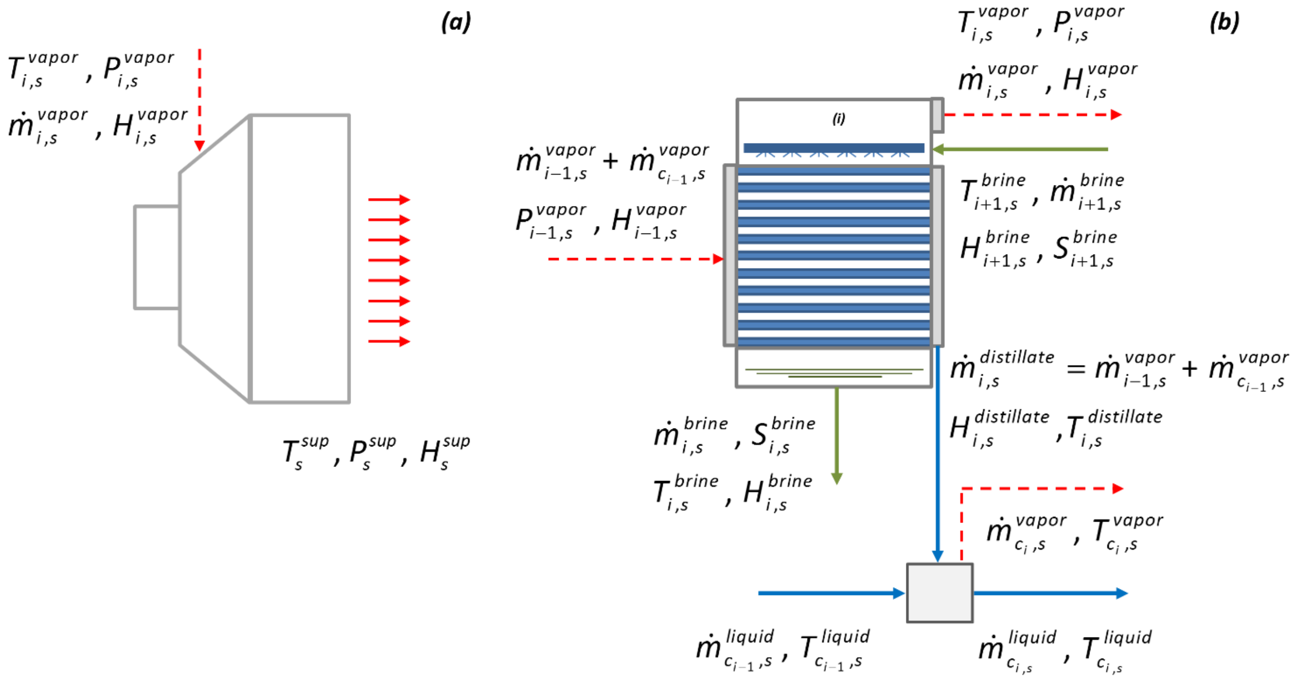

Figure 2. Decision variables for the optimization of: (*a*) single-stage compressor; and, (*b*) effect *i* of the horizontal falling film evaporator coupled to flashing tank *i* in the MEE-MVR system

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Two stage stochastic model

Mathematical modelling approach

Design of the multiple-effect evaporator

1. Mass balances

Evaporator effect *i*:

$$\dot{m}_{i+1,s}^{brine} = \dot{m}_{i,s}^{brine} + \dot{m}_{i,s}^{vapor} \qquad \forall 1 \le i \le I-1,\ \forall s \in S$$

$$\dot{m}_{i+1,s}^{brine} \cdot S_{i+1,s}^{brine} = \dot{m}_{i,s}^{brine} \cdot S_{i,s}^{brine} \qquad \forall 1 \le i \le I-1,\ \forall s \in S$$

First effect:

$$\tilde{m}_{in,s}^{feed} = \dot{m}_{i,s}^{brine} + \dot{m}_{i,s}^{vapor} \qquad \forall i = I,\ \forall s \in S$$

$$\tilde{m}_{in,s}^{feed} \cdot \tilde{S}_{in,s}^{feed} = \dot{m}_{i,s}^{brine} \cdot S_{i,s}^{brine} \qquad \forall i = I,\ \forall s \in S$$

$$\left.\begin{array}{l}\tilde{m}_{in,s}^{feed} \\ \tilde{S}_{in,s}^{feed}\end{array}\right\}$$ are the stochastic parameters that define flowrate and salinity for the feed water in the set of distinct scenarios

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Mathematical modelling approach

Design of the multiple-effect evaporator

2. Global energy balances

$$Q_{i,s} + \dot{m}_{i+1,s}^{brine} \cdot H_{i+1,s}^{brine} = \dot{m}_{i,s}^{brine} \cdot H_{i,s}^{brine} + \dot{m}_{i,s}^{vapor} \cdot H_{i,s}^{vapor} \qquad \forall i < I,\ \forall s \in S$$

$$Q_{i,s} + \tilde{m}_{in,s}^{feed} \cdot H_{i,s}^{feed} = \dot{m}_{i,s}^{brine} \cdot H_{i,s}^{brine} + \dot{m}_{i,s}^{vapor} \cdot H_{i,s}^{vapor} \qquad \forall i = I,\ \forall s \in S$$

specific enthalpies are estimated at the same boiling point temperature

3. Boiling point temperature

$$T_{i,s}^{boiling} = T_{i,s}^{ideal} + BPE_{i,s} \qquad \forall i \in I,\ \forall s \in S$$

$$BPE_{i,s} = \begin{bmatrix} 0.1581 + 2.769 \cdot \left(X_{i,s}^{salt}\right) - 0.002676 \cdot \left(T_{i,s}^{ideal}\right) \\ + 41.78\left(X_{i,s}^{salt}\right)^{0.5} + 0.134 \cdot \left(X_{i,s}^{salt} \cdot T_{i,s}^{ideal}\right) \end{bmatrix} \qquad \forall i \in I,\ \forall s \in S$$

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Mathematical modelling approach

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Design of the multiple-effect evaporator

4. Energy requirements

$$Q_{i,s} = \dot{m}_s^{sup} \cdot Cp_{i,s}^{vapor} \cdot \left(T_s^{sup} - T_{i,s}^{condensate} \right) + \dot{m}_s^{sup} \cdot \left(H_{i,s}^{cv} - H_{i,s}^{condensate} \right) + Q_s^{external} \quad \forall i = 1, \ \forall s \in S$$

$$Q_{i,s} = \left(\dot{m}_{i-1,s}^{vapor} + \dot{m}_{c_{i-1,s}}^{vapor} \right) \cdot \lambda_{i,s} \quad \forall i > 1, \ \forall s \in S$$

In which,

$$Q_s^{external} = \dot{m}_s^{steam} \cdot Cp_s^{vapor} \cdot \left(T_s^{steam} - T_{i,s}^{condensate} \right) + \dot{m}_s^{steam} \cdot \left(H_{i,s}^{cv} - H_{i,s}^{condensate} \right) \quad \forall i = 1, \ \forall s \in S$$

energy amount from the external source (steam) used to avoid oversized equipment

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Design of the multiple-effect evaporator

5. Heat transfer area

$$A^{evaporator} = \sum_{i=1}^{I} A_i$$

In which,

$$A_i \geq \begin{bmatrix} \dot{m}_s^{sup} \cdot Cp_{i,s}^{vapor} \cdot \left(T_s^{sup} - T_{i,s}^{condensate}\right) \Big/ \left(U^S \cdot LMTD_{i,s}\right) \\ + \dot{m}_s^{sup} \cdot \left(H_{i,s}^{cv} - H_{i,s}^{condensate}\right) \Big/ U_{i,s} \cdot \left(T_{i,s}^{condensate} - T_{i,s}^{boiling}\right) \end{bmatrix} \quad \forall i = 1,\ \forall s \in S$$

$$A_i \geq Q_{i,s} \Big/ \left(U_{i,s} \cdot LMTD_{i,s}\right) \qquad \forall i > 1,\ \forall s \in S$$

Overall heat transfer coefficient:

$$U_{i,s} = 0.001 \cdot \begin{bmatrix} 1939.4 + 1.40562 \cdot \left(T_{i,s}^{boiling}\right) \\ -0.00207525 \cdot \left(T_{i,s}^{boiling}\right)^2 + 0.0023186 \cdot \left(T_{i,s}^{boiling}\right)^3 \end{bmatrix} \quad \forall i > 1,\ \forall s \in S$$

Log mean temperature difference :

$$LMTD_{i,s} = \left[0.5 \cdot \left(\theta_{1i,s} \cdot \theta_{2i,s}\right) \cdot \left(\theta_{1i,s} + \theta_{2i,s}\right)\right]^{\frac{1}{3}} \quad \forall i \in I,\ \forall s \in S$$

$$\theta_{1i,s} = \begin{cases} T_s^{sup} - T_{i,s}^{boiling} & \forall i = 1,\ \forall s \in S \\ T_{i,s}^{sat} - T_{i,s}^{boiling} & \forall i > 1,\ \forall s \in S \end{cases} \quad \text{and}$$

$$\theta_{2i,s} = \begin{cases} T_{i,s}^{condensate} - T_{i+1,s}^{boiling} & \forall i = 1,\ \forall s \in S \\ T_{i,s}^{sat} - T_{i+1,s}^{boiling} & \forall 1 < i < I,\ \forall s \in S \\ T_{i,s}^{sat} - T_{i,s}^{feed} & \forall i = I,\ \forall s \in S \end{cases}$$

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Two stage stochastic model

Mathematical modelling approach

Design of the multiple-effect evaporator

6. Pressure feasibility

$$P_{i,s}^{vapor} \geq P_{i+1,s}^{vapor} + \Delta P_{\min} \qquad \forall i < I,\ \forall s \in S$$

7. Constraints on temperature

$$T_s^{sup} \geq T_{i,s}^{condensate} + \Delta T_{\min}^{1} \qquad \forall i = 1,\ \forall s \in S$$

$$T_{i-1,s}^{boiling} \geq T_{i,s}^{condensate} + \Delta T_{\min}^{1} \qquad \forall i > 1,\ \forall s \in S$$

$$T_{i,s}^{boiling} \geq T_{i+1,s}^{boiling} + \Delta T_{\min}^{2} \qquad \forall i < I,\ \forall s \in S$$

$$T_{i,s}^{boiling} \geq T_{i,s}^{feed} + \Delta T_{\min}^{2} \qquad \forall i = I,\ \forall s \in S$$

$$T_{i,s}^{condensate} \geq T_{i+1,s}^{boiling} + \Delta T_{\min}^{3} \qquad \forall i < I,\ \forall s \in S$$

$$T_{i,s}^{condensate} \geq T_{i,s}^{feed} + \Delta T_{\min}^{3} \qquad \forall i = I,\ \forall s \in S$$

$$T_{i,s}^{condensate} \geq T_{i,s}^{boiling} + \Delta T_{\min}^{4} \qquad \forall i \in I,\ \forall s \in S$$

$$T_{i,s}^{sat} \geq T_{i,s}^{boiling} + \Delta T_{\min}^{4} \qquad \forall i \in I,\ \forall s \in S$$

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Two stage stochastic model

Mathematical modelling approach

Design of the mechanical vapor compressor

1. Isentropic temperature

$$T_s^{is} = \left(T_{i,s}^{mix} + 273.15\right)\cdot\left(P_s^{sup} / P_{i,s}^{vapor}\right)^{\frac{\gamma-1}{\gamma}} - 273.15 \qquad \forall i = I,\ \forall s \in S$$

In which,

$$P_s^{sup} \le CR_{\max} \cdot P_{i,s}^{vapor} \qquad \forall i = I\ ,\ \forall s \in S$$

2. Superheated vapor temperature

$$T_s^{sup} = T_{i,s}^{mix} + \frac{1}{\eta_s}\cdot\left(T_s^{is} - T_{i,s}^{mix}\right) \qquad \forall i = I,\ \forall s \in S$$

↑

isentropic efficiency

3. Isentropic efficiency

$$\eta_s = \left(0.35/0.8\right)\cdot\left(\frac{W_s}{WC} - 0.2\right) + 0.5 \qquad \forall s \in S$$

In which,

$$WC \ge W_s \qquad \forall s \in S$$

These equations are valid for:

$$0.5 \le \eta_s \le 0.85 \qquad\qquad 0.2 \le \frac{W_s}{WC} \le 1$$

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Two stage stochastic model

Mathematical modelling approach

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Two stage stochastic model

Mathematical modelling approach

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Design of the mechanical vapor compressor

4. Compression work

$$W_s = \dot{m}_s^{sup} \cdot \left(H_s^{sup} - H_{i,s}^{vapor} \right) \qquad \forall i = I,\ \forall s \in S$$

5. Constraints on temperature and pressure

$$T_s^{sup} \geq T_{i,s}^{mix} \qquad \forall i = I,\ \forall s \in S$$

$$P_s^{sup} \geq P_{i,s}^{vapor} \qquad \forall i = I,\ \forall s \in S$$

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Design specification for ZLD operation

ZLD operation is ensured by the following constraint:

$$S_{i,s}^{brine} \geq S^{design} \qquad \forall i = 1,\ \forall s \in S$$

In this case,

$$S^{design} = 300\ g\ kg^{-1}\ \text{TDS}$$

The inclusion of this constraint in the model restricts the search space to solutions that meet a minimum salinity requirement for the bine (*i.e.*, brine salinity close to salt saturation conditions)

Lower costs are expected for weaker brine salinity restrictions

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Mathematical modelling approach

Stochastic objective function

The stochastic objective function for the minimization of the expected total annualized cost is given by:

$$\min \quad TAC^{Exp} = \sum_{s \in S} \left(prob_s \right) \cdot TAC_s = \sum_{s \in S} \left(prob_s \right) \cdot \left(CAPEX + OPEX_s \right)$$

$$\text{s.t.} \quad \text{all equality and inequality constraints}$$

In which, the distributions of capital investment and operational costs are given by:

$$CAPEX = fac \cdot \left(\frac{CEPCI^{2015}}{CEPCI^{2003}} \right) \cdot \left[\begin{array}{l} \left(C_{PO} \cdot F_{BM} \cdot F_P \right)^{evaporator} + \left(C_{PO} \cdot F_{BM} \cdot F_P \right)^{compressor} + \\ \left(\sum_{i=1}^{I} C_{POi} \cdot F_{BM} \cdot F_P \right)^{flash} + \left(C_{PO} \cdot F_{BM} \cdot F_P \right)^{preheater} \end{array} \right]$$

$$OPEX_s = C^{electricity} \cdot W_s + C^{steam} \cdot Q_s^{external}$$

Observations:

- The resulting formulation was implemented in GAMS (version 24.8.5) and solved with the interior-point local solver IPOPT (with CPLEX sub-solver)
- The CPU time for stochastic optimizations did not exceed 60 s
- The MEE-MVR system should operate at low temperatures and pressures to avoid rusting

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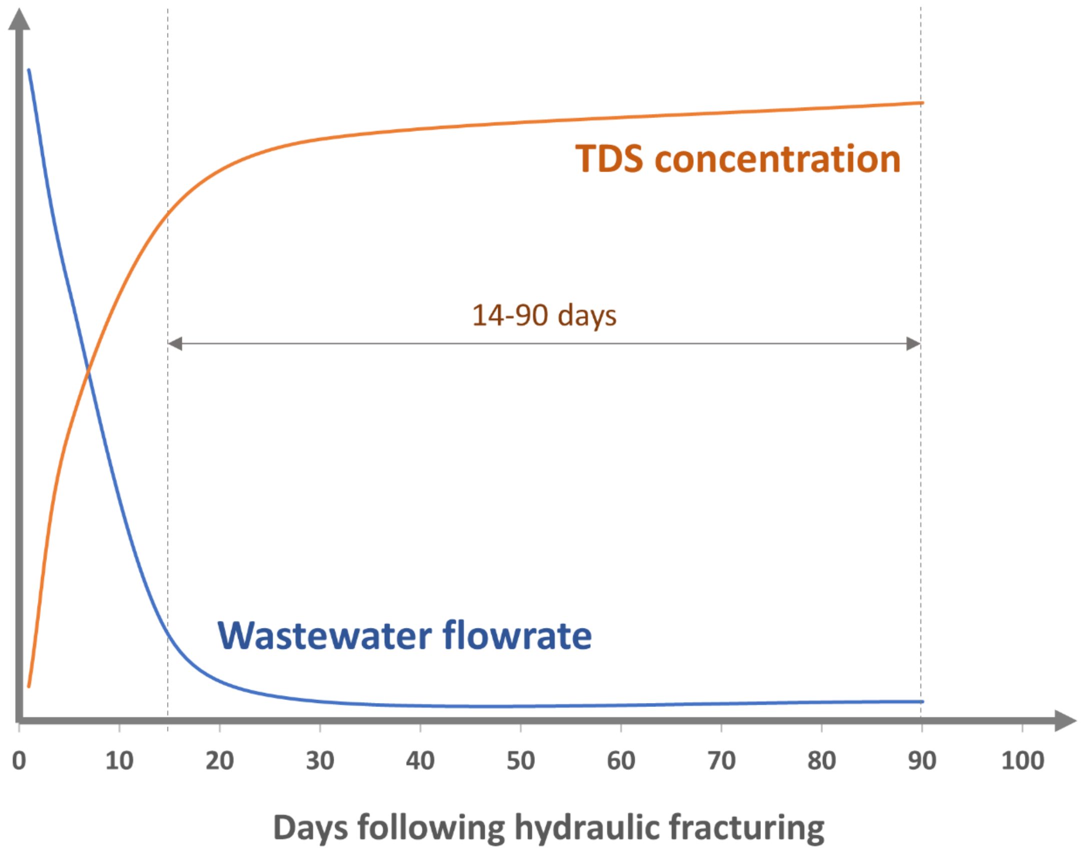
Two stage stochastic model

Scenarios generation



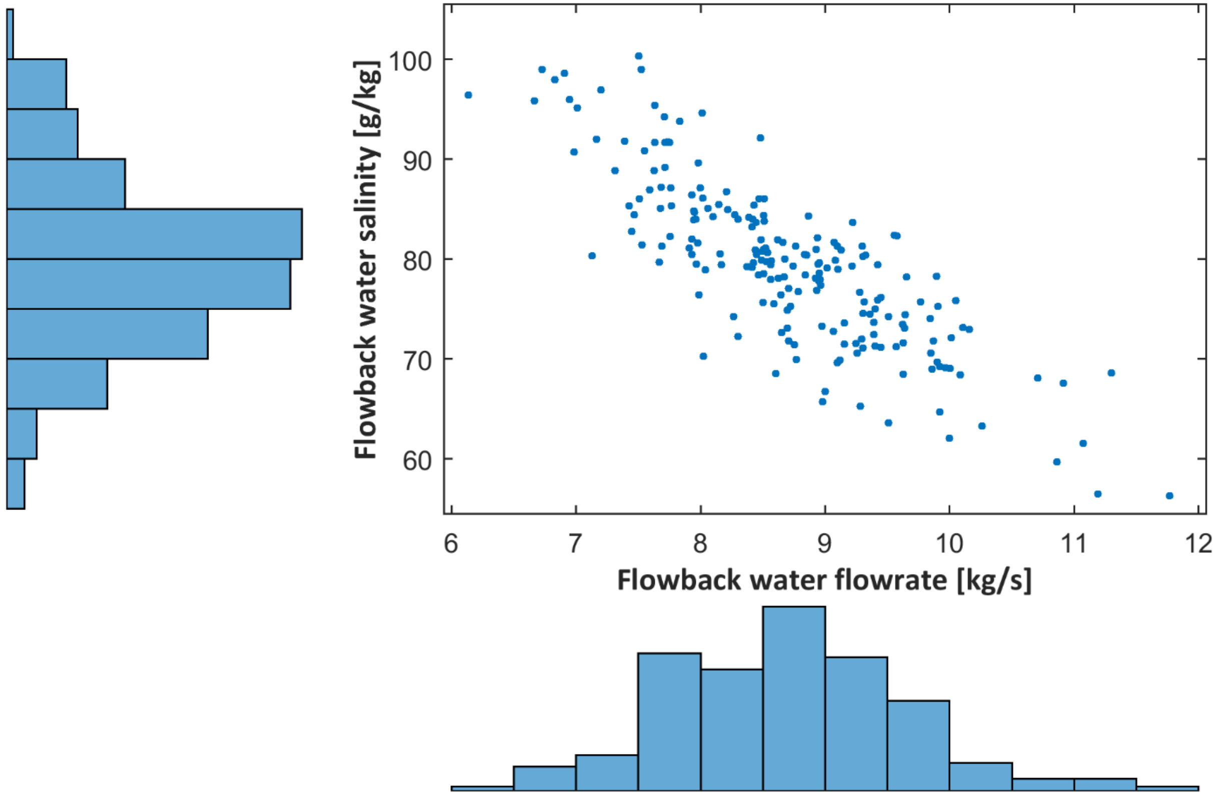


Figure 3. Correlated feeding scenarios generated with marginal normal distribution, considering matrix correlation of -0.8 and standard deviation of 10% from expected mean values (200 scenarios)

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Case study

Shale gas wastewater desalination

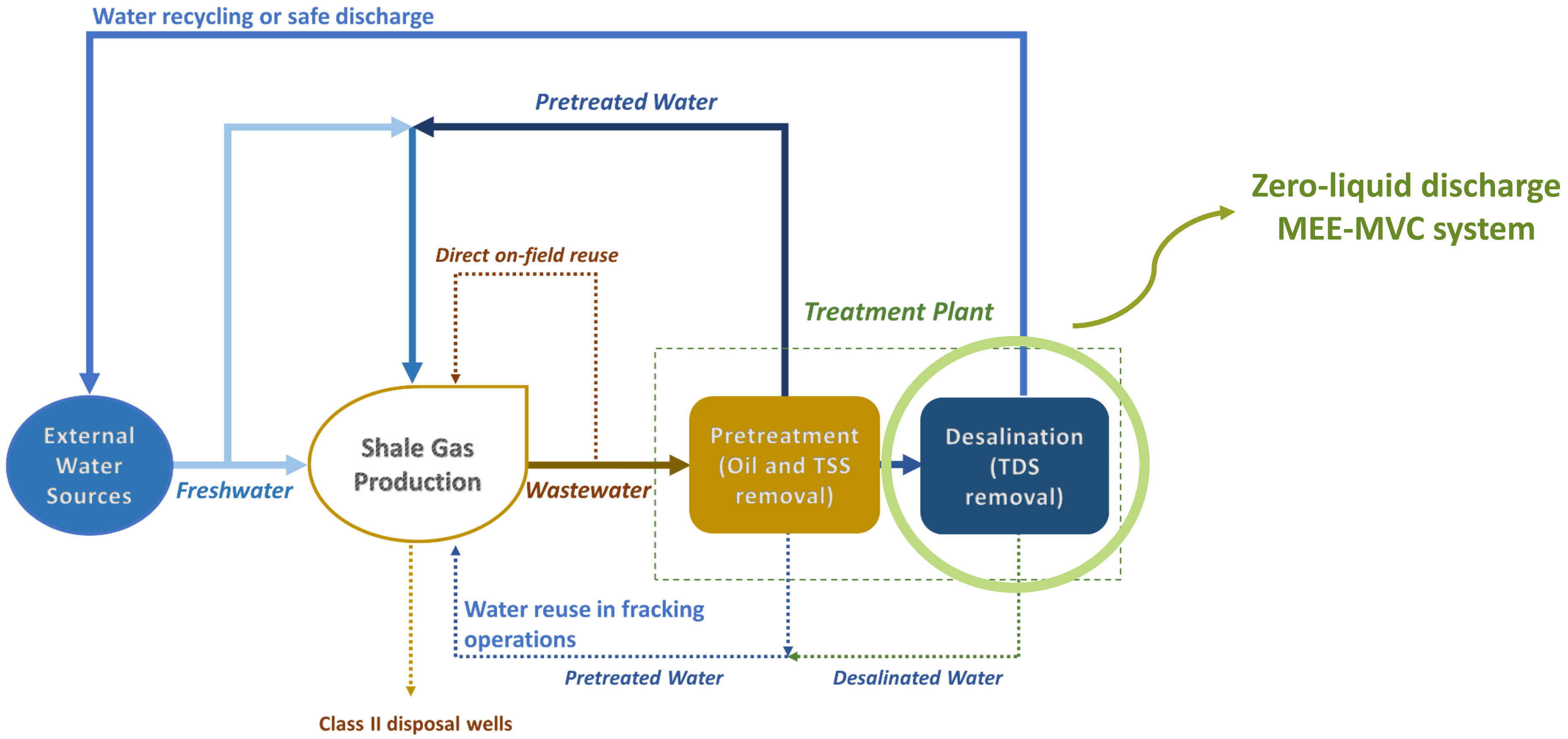

Figure 4. Wastewater management alternatives for shale gas industry

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[>>COnCEPT] Computer Optimization in Chemical Engineering Processes and Technologies
Universitat d'Alacant Universidad de Alicante

ESCAPE-27 Barcelona October 1st - 5th 2017 European Symposium on Computer-Aided Process Engineering
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Case study

Shale gas wastewater desalination

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Table 1. Problem data for the case study regarding the optimal design of MEE-MVR desalination systems under well data uncertainty

Feed water	Expected mean value for mass flowrate, (kg s^{-1})	8.68
	Temperature, (ºC)	25
	Expected mean value for salinity, (g kg^{-1} or k ppm)	80
Mechanical vapor compressor	Isentropic efficiency, (%)	50–85
	Heat capacity ratio	1.33
	Maximum compression ratio	3
Process specification and restrictions	Brine salinity for ZLD operation, (g kg^{-1} or k ppm)	300
	Maximum effect temperature, (ºC)	100
	Maximum effect pressure, (kPa)	200
Cost data	Electricity cost [a], (US$ (kW year)$^{-1}$)	850.51
	Steam cost, (US$ (kW year)$^{-1}$)	418.80
	Fractional interest rate per year	0.1
	Amortization period	10
	Working hours per year	8760

Standard deviations: 5, 10 and 20 %

Matrix correlation: –0.7

[a] *Cost data obtained from Eurostat database (European Commission, 2016)*

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Case study

Shale gas wastewater desalination

Deterministic solution:

TAC: 1055 kUS$ year^{-1}

OPEX: 463 kUS$ year^{-1}

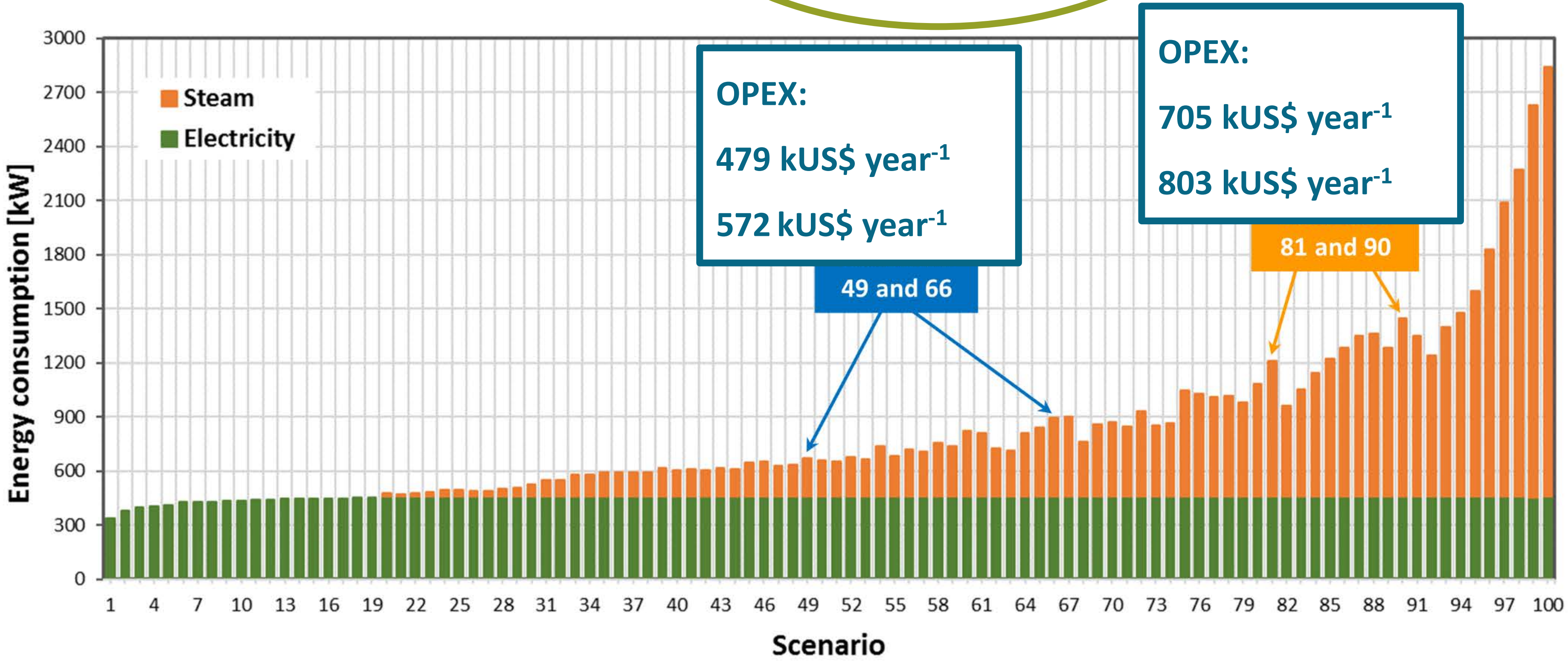

Figure 5. Energy consumption distribution throughout the different feeding scenarios, obtained via stochastic approach with fixed equipment capacities as provided by the deterministic solution

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Case study

Shale gas wastewater desalination

~6.8 US$ per cubic meter (~0.03 US$ gallon^{-1})

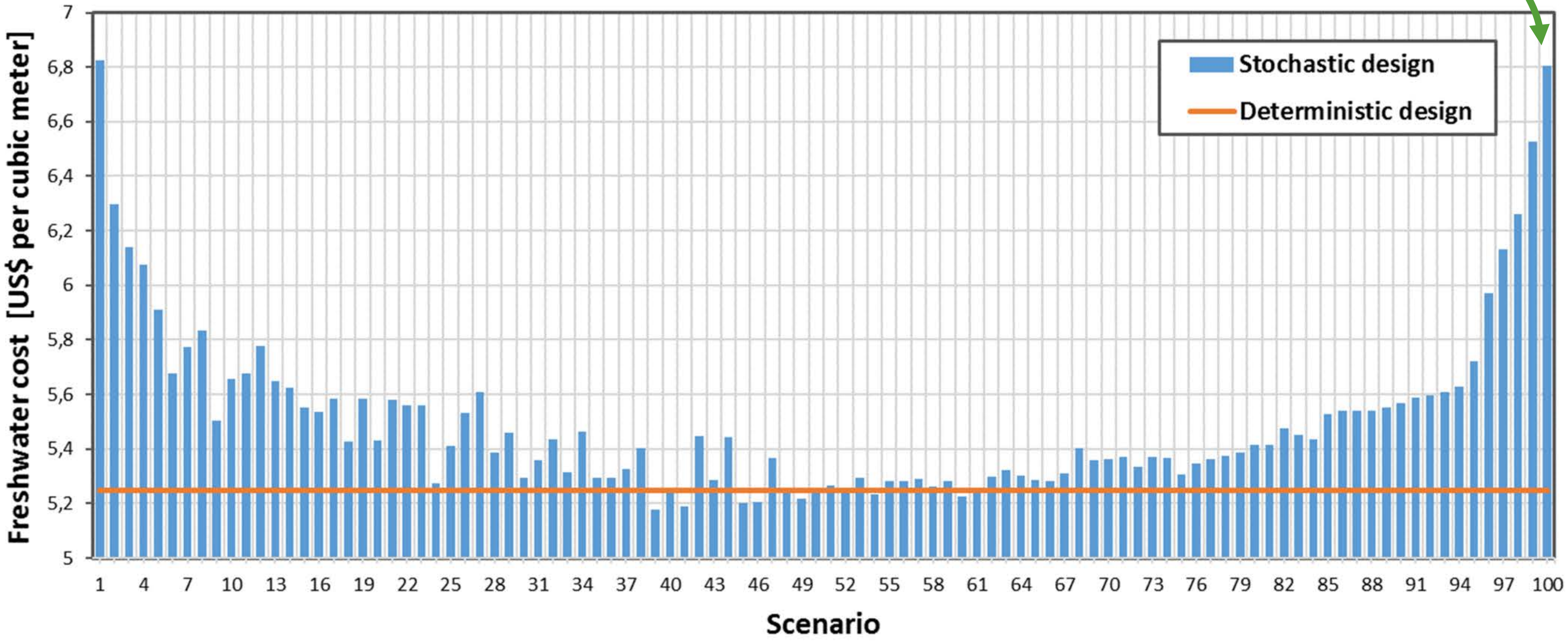

Figure 6. Freshwater cost distribution throughout the different feeding scenarios, obtained via stochastic approach with fixed equipment capacities as provided by the deterministic solution

This value correspond to an increase of ~30% in comparison with the deterministic solution

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Case study

Shale gas wastewater desalination

~3.8 US$ per cubic meter (~0.02 US$ gallon^{-1})

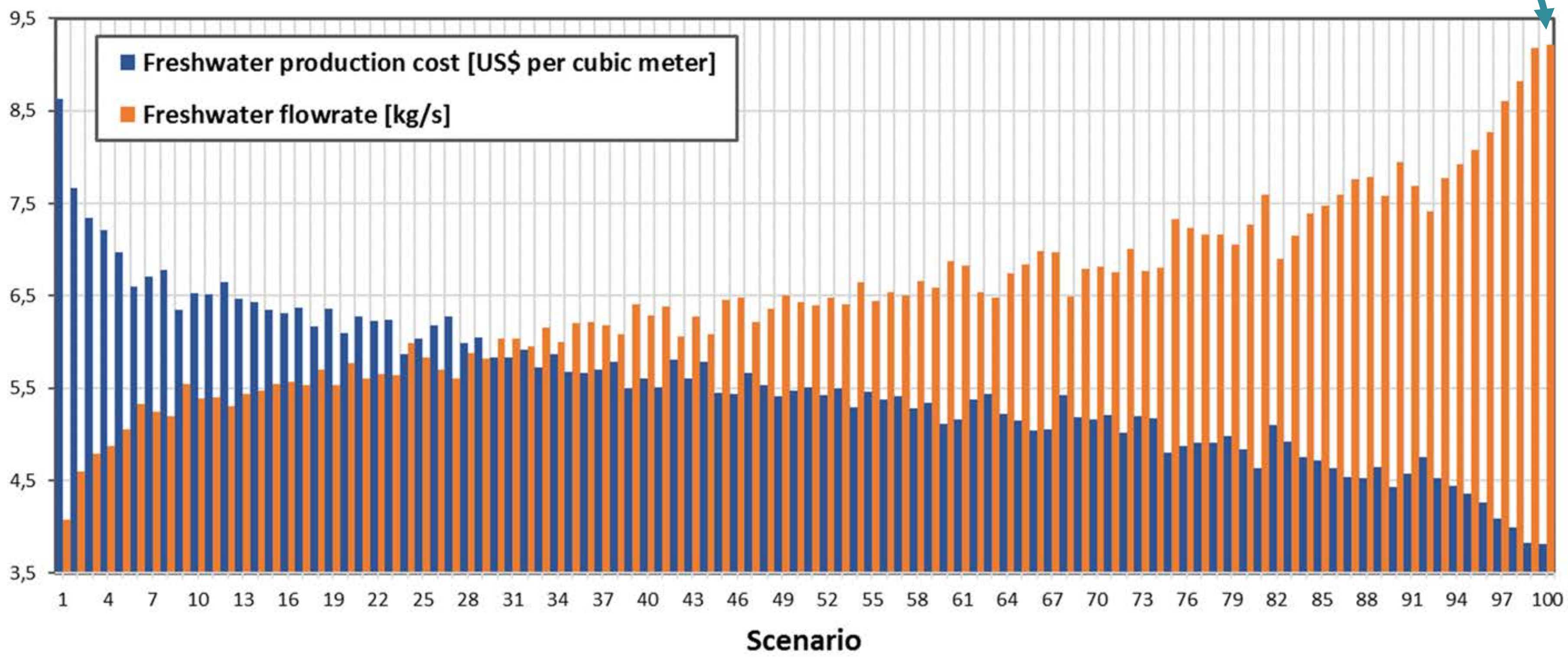

Figure 7. Distributions of freshwater production cost and produced freshwater obtained by the stochastic model throughout the distinct feeding scenarios

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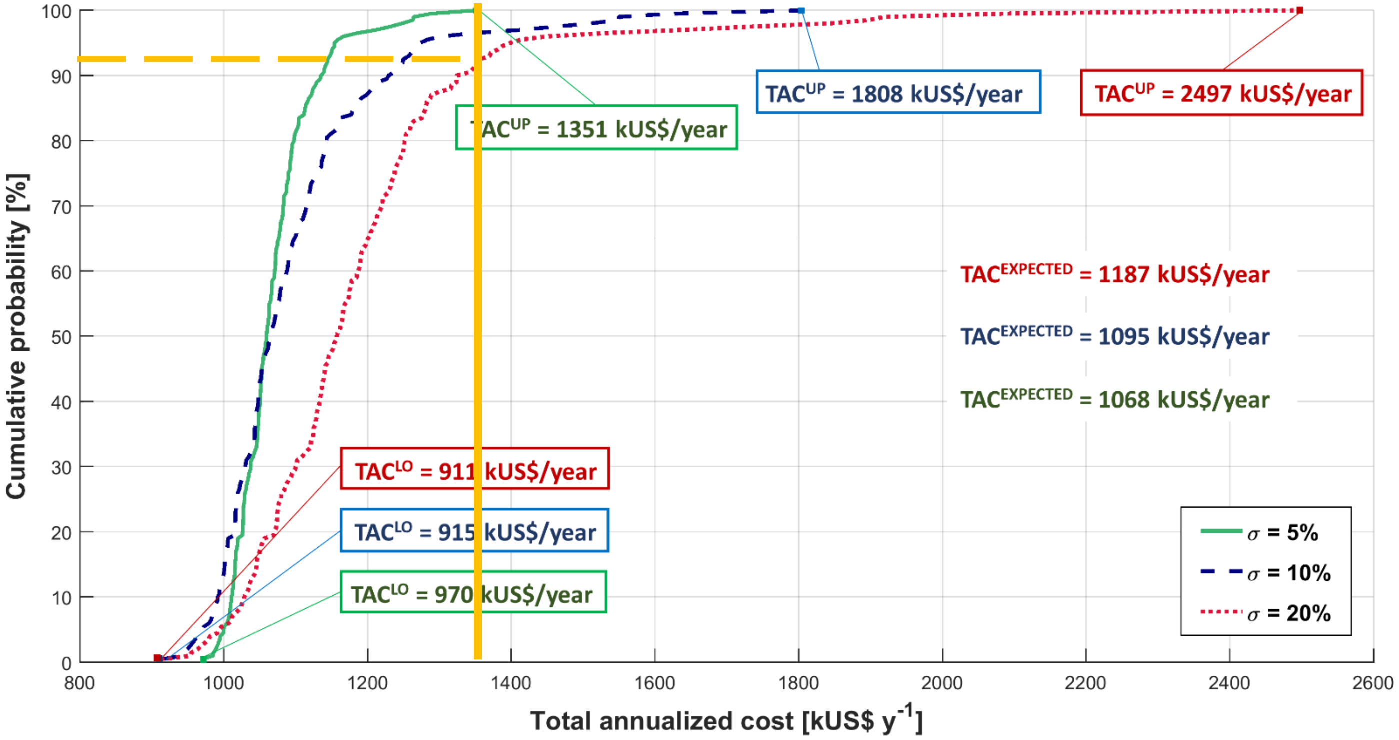
Case study

Shale gas wastewater desalination

20% curve presents ~8% of probability of exceeding the target cost of 1351 kUS$ year^{-1}, while this probability is null for the 5% curve



Higher standard deviations imply riskier decision-making

Figure 8. Cumulative probability curves for the ZLD system economic performance under consideration of correlated uncertain parameters (matrix correlation of 0.7)

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Remarks

Overview

- A new stochastic multiscenario optimization model is introduced for the robust design of ZLD desalination systems under uncertainty
- Flowback water salinity and flowrate are both considered as uncertain design parameters
- These uncertain parameters are mathematically modelled as a set of correlated scenarios with given probability of occurrence
- The correlated scenarios are generated from a multivariate normal distribution via Monte Carlo sampling technique with a symmetric correlation matrix
- For ensuring the goal of ZLD operation in the uncertain space, we define the discharge brine salinity close to salt saturation condition as a design constraint for all feeding scenarios
- The resulting stochastic multiscenario NLP-based model is implemented in GAMS, and optimized by the minimization of the expected total annualized cost of the desalination process

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Remarks

Conclusions

- Comparative results between deterministic and stochastic (with fixed deterministic solution) approaches indicate that operational expenses can be prohibitive for some correlated scenarios
- This is because the ZLD process is not able to provide all system flexibility required against feeding variability conditions
- These results highlight the importance of the proposed stochastic model to optimize systems subjected to design parameters uncertainty
- Furthermore, cumulative probability curves show that higher standard deviations for uncertain parameters imply riskier decision-making
- This is a consequence of their increased probability of exceeding a target total annualized cost
- The results obtained can be used to support decision-makers towards the implementation of more robust and reliable ZLD desalination systems in the shale gas industry

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Thank you for your attention!

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