# **DYNAMIC MODELLING AND SIMULATION: NON-EQUILIBRIUM EFFECTS AND HEAT TRANSFER**

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### **Summary**

This chapter addresses two topics related to the thermal efficiency of MSF desalination plants: non-equilibrium effects and discrepancies between the nominal and the observed heat transfer situations.

Non-equilibrium is addressed first by focusing on simulation models where the tradeoff between model complexity and prediction accuracy is of major relevance. Based on measured data from a 20 stage industrial-size MSF desalination plant it is shown that accounting for non-equilibrium in a simulation model is insignificant. This is due to the fact that uncertainties prevailing in the measurements as obtained from common industrial plant instrumentation are in the same order of magnitude as one expects the non-equilibrium temperature losses. The insignificance of non-equilibrium is also illustrated by presenting dynamic simulation results obtained from an equilibrium model in comparison to those obtained from a model including a state-of-the art correlation to predict non-equilibrium temperature losses. These findings need to be clearly distinguished from the design problem where the relation between non-equilibrium losses and stage design parameters is of key interest.

Modeling of the heat transfer is addressed in the second part of this article. The heat transfer situation as observed during plant operation deviates from the nominal situation due to scaling on the tube side and due to non-condensible gases on the shell side. Both effects are not accounted for in the model since validated formulas to calculate scale formation or the release of non-condensible gases are lacking. It is shown that due to the non-condensible gases a compensation for non-idealities in the heat transfer must depend on the plant operating conditions if one expects predictions of reasonable

accuracy from the simulation model. Therefore, the typical approach for compensation by means of constant fouling factors cannot be applied.

### 1. Introduction

Non-equilibrium in MSF desalination occurs due to incomplete flashing of the liquid brine in the evaporator stages. Although the brine approaches thermal equilibrium as it evaporates and flows towards the stage exit, a residual superheat is commonly present at the stage exit. A certain loss of thermal efficiency is associated with this behavior since less heat is recovered at higher temperatures.

As the rate of evaporation is integrally linked to the fluid dynamics as well as to mass and heat transfer phenomena, a rigorous non-equilibrium model for the liquid brine is extremely complex to derive. First steps in that direction were undertaken by Miyatake et al. (1993), who applied an empirical correlation to determine the rate of evaporation along the streamlines found from two-dimensional CFD simulations.

The approach to equilibrium is commonly quantified by means of an efficiency variable, the non-equilibrium temperature loss, which is of great interest for plant design since the objectives of economic stage design and high thermal efficiency often coincide.

Consequently, much effort has been spent on predicting the non-equilibrium temperature loss in MSF plants. Lior (1986) compares various correlations available in the literature and concludes that they yield highly differing results. This indicates the difficulties in generally predicting the non-equilibrium temperature loss in MSF desalination plants.

Although the prediction of the non-equilibrium temperature loss gives valuable support during plant design its role for plant simulation still needs to be defined. During plant design one is mainly interested in the relationship between stage geometry and the nonequilibrium temperature loss. In contrast, the tradeoff between model complexity and its prediction accuracy is of major importance for simulation models. Consequently, nonequilibrium temperature losses might not be as relevant for plant simulation as they are for plant design.

Based on the experimental findings from an industrial-size MSF desalination plant, the relevance of non-equilibrium temperature losses in a simulation model with respect to the achievable model accuracy is addressed in the first part of this article.

The second part of this article deals with the heat transfer situation as observed during the tests on the industrial-size reference plant. Of course, the observed situation differs from the nominal situation that can be calculated from validated and widely applied formulas. This is due to scaling in the heat exchanger tubes and due to non-condensable gases on the shell side. Consequently, some correction of the nominal heat transfer coefficients is required in order to meet the observed situation. For MSF plant design, this is accomplished by the fouling factors that compensate for both of the aforementioned additional heat transfer resistances In order to choose a sufficiently large heat exchanger surface, the additional heat transfer resistances are commonly rather overestimated. Whether such an empirical correction which is independent of plant operating conditions can give rise to satisfactory results in a simulation model is reviewed.

## 2. Non-equilibrium Effects

A very efficient way to treat non-equilibrium effects is to compensate the equilibrium model by an efficiency factor such as the Murphree efficiency factor which is commonly applied for distillation columns. Other more sophisticated modeling approaches for non-equilibrium strive for a physical description of the mass and heat transfer over the phase boundary through appropriate transport laws.

In MSF desalination, non-equilibrium is considered a relevant phenomenon. Due to incomplete flashing the liquid brine leaves an evaporator stage at a higher temperature than the corresponding equilibrium temperature. This involves a certain loss of energy since less heat of evaporation is transferred to the cooling brine at high brine temperatures. Consequently, non-equilibrium decreases the thermal efficiency of the MSF process.

## 2.1. Non-equilibrium Temperature Loss

In a mathematical MSF plant model non-equilibrium is expressed by means of an efficiency variable, the non-equilibrium temperature loss  $\Delta'$  which defines the superheat of the brine due to incomplete flashing. It is defined as the difference between the liquid brine temperature ( $T_B$ ) and the temperature of the emanating vapor ( $T_V$ ) which is also the boiling point temperature of the liquid brine at the flashing chamber pressure. Hence,



Figure 1. Stage temperature schematic.

see also Figure 1 for the location of the stage temperatures. Consequently, the non-equilibrium temperature loss approaches zero as the flashed brine approaches its boiling

point temperature. It may be noted here that  $\Delta'$  is sometimes also referred to as the non-equilibrium temperature difference or the non-equilibrium allowance.

One now attempts to relate the temperature of the emanating water  $(T_V)$  to a well measurable process quantity which is the condensation temperature in the distillate chamber  $(T_D)$ . It is expected to be lower than the temperature of the emanating water due to the absence of dissolved solids in the distillate chamber. In terms of the simplified physical property functions commonly applied in MSF plant models, this can be expressed by means of the boiling point elevation (*BPE*)

$$T_V = T_D + BPE$$

(2)

if the small pressure losses across the demister and in the heat exchanger tubes are neglected which is common practice for the definition of the non-equilibrium temperature loss.

### 2.2. Empirical Correlations for the Non-equilibrium Temperature Loss

A large number of empirical correlations to predict the non-equilibrium temperature loss have been proposed in the literature. A comprehensive overview is given by Lior (1986), who shows the highly differing predictions of the investigated correlations for a given stage configuration.

These correlations are typically applied for plant design where an economic stage design with least chamber length often coincides with the demand for a high evaporation efficiency with small non-equilibrium temperature losses. Since the focus of this article is (dynamic) MSF plant simulation rather than plant design, only one typical correlation for the non-equilibrium temperature loss is presented in the following. It serves as a representative example for the many correlations applied for plant design.

Recently, Rautenbach et al. (1996), suggested an empirical non-equilibrium correlation that was shown to correspond accurately to laboratory scale experimental data as well as to the predictions of some other published non-equilibrium correlations. It relates the non-equilibrium temperature loss to the brine inflow temperature, the vapor pressure difference, the brine flowrate, the brine level and to the stage length and width in the following way:

$$\Delta^{\prime(i)} = 50.7 \left(T_B^{(i-1)}\right)^{-2.0} \left(p^{(i-1)} - p^{(i)}\right)^{0.71} \left(\frac{m_{Bin}^{(i)}}{B^{(i)}}\right)^{0.07} \left(l^{(i)}\right)^{1.1} \left(L^{(i)}\right)^{-1.01}$$
(4)

The superscripts (i) and (i-1) indicate the stage number of the process quantities. See Table 1 for the exact definition of the symbols and their units of measurement.

$\alpha_{steam}$	Steam side heat transfer coefficient	$kW m^{-2} K^{-1}$
$\alpha_{water}$	Water side heat transfer coefficient	$kW m^{-2} K^{-1}$

$\Delta'$	Non-equilibrium temperature loss	С
B	Stage width	m
BPE	Boiling point elevation	С
FF	Fouling factor	$kW m^{-2} K^{-1}$
k <sub>clean</sub>	Overall heat transfer coefficient under clean conditions	$kW m^{-2} K^{-1}$
k <sub>true</sub>	Overall heat transfer coefficient under operating conditions	$kW m^{-2} K^{-1}$
L	Brine level	m
L	Stage length	m
<i>m</i> <sub>Bin</sub>	Brine inlet flowrate	kg s <sup>-1</sup>
Р	Vapor pressure	$N m^{-2}$
$T_B$	Brine temperature	С
$T_D$	Condensation temperature in the distillate	С
	chamber	
$T_{v}$	Temperature of emanating vapor in the flashing	С
	chamber	
<i>(i)</i>	Process quantity on stage i	
( <b>I-1</b> )	Process quantity on stage i-1	

### Table 1. List of symbols.

According to Rautenbach et al. (1996), this correlation is capable of predicting the laboratory scale measurements with an average deviation of 0.29°C. However, since it is based on experiments in a low temperature range of the brine between 19°C and 58°C the authors state that extrapolation to higher temperature should be done with caution.



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