CHEMICAL ENGINEERING TRANSACTIONS
VOL. 81, 2020

A publication of AIDIC
The Italian Association of Chemical Engineering
Online at www.cetjournal.it

Guest Editors: Petar S. Varbanov, Qiuwang Wang, Min Zeng, Panos Seferlis, Ting Ma, Jiří J. Klemeš

ISBN 978-88-95608-79-2; **ISSN** 2283-9216

DOI: 10.3303/CET2081122

Optimisation and Analysis Based on Bi-Level Reduced-Order Model for Coupled Heat and Mass Transfer Processes Under Uncertainty

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This work proposes an integrated framework to build fast and high-fidelity bi-level reduced-order models (ROMs) for heat and mass transfer processes systems. In the proposed framework, the bi-level ROMs including the ROM for output variables (yROM) and the ROM for state variables (zROM) corresponding to its input variables of the systems are developed by integrating principal component analysis (PCA) with artificial neural networks (ANN), which can closely approximate the results of computational fluid dynamics (CFD). In particular, the CPU time is significantly reduced with the fast bi-level ROMs. A case study is used to demonstrate the benefits of using our proposed bi-level ROMs methodology for simulation and optimisation for heat and mass transfer processes systems, where a bi-level ROMs for the closed wet cooling towers (CWCTs) is built with the help of exergy analysis. The design points served for CFD simulations are randomly sampled by stochastic reduced-order modelling (SROM). The developed yROM is used for stochastic optimisation of exergy efficiency ratio and then the corresponding optimal exergy flux fields are then reconstructed and analysed based on zROM.

1. Introduction

Coupled heat and mass transfer between humid air and liquid is the most common and fundamental process in heating, ventilating, and air conditioning (HVAC) systems such as closed wet cooling tower (CWCT). The heat and mass transfer process in the CWCTs relies on the evaporative heat transfer of the falling film outside the serpentine coils to achieve the required cooling target of the tower. In principle, a variety of parameters (design, structure, and operation parameters) can affect the thermodynamic performances of a specific thermal system. For example, the influence of different kinds of tubes (plain, oval, longitudinal fin) (Xie et al., 2017) and arrangement (staggered tube bundles) (Xie et al., 2019) on the performance of the CWCT were deciphered. Especially, note that the daily operation of a cooling tower is directly affected by the fluctuating environmental parameters. Systematic investigation on heat and mass transfer processes under uncertainty will help researchers and engineers to gain a better understanding of the internal operation status and have an opportunity to improve the design of CWCTs.

Exergy (or availability) analysis has been widely used for the analysis and optimisation of the HVAC systems. It can quantitatively and qualitatively exploit the nature of energy utilisation from the perspective of the second law of thermodynamics. Over the past decades, researchers have dedicated to improving the thermodynamic performance of cooling towers and significant studies have been reported in the literature based on exergy analysis. Ren et al. (2002) analytically reviewed principles of exergy analysis in HVACs and unusually selected saturated atmospheric air for the dead state which makes it easier to evaluate the theoretical limit of evaporative cooling capacity. Qureshi et al. (2007) conducted a thermodynamic analysis of counter flow wet cooling tower and evaporative heat exchangers, and the influence of various input parameters on second-law efficiency and exergy destruction is investigated. It is of great importance to observe and display the internal thermal phenomena in multidimensional state space for equipment design and flow field analysis which further results in thermodynamic improvements and process intensification. However, the previous studies on exergy analysis are mainly conducted from the perspective of the information of input/output streams connected with the

Paper Received: 22/04/2020; Revised: 07/06/2020; Accepted: 17/06/2020
Please cite this article as: Qu J., Liu H., Pan M., Zhang B., Chen Q., He C., 2020, Optimisation and Analysis Based on Bi-Level Reduced-Order Model for Coupled Heat and Mass Transfer Processes Under Uncertainty, Chemical Engineering Transactions, 81, 727-732 DOI:10.3303/CET2081122

systems. In other words, these studies only focused on analysing the lumped parameters of exergy flows but ignored the exploration of spatially distributed exergy parameters in flow fields inside the equipment.

It is not easy to get practical models of distributed parameter thermal systems which can be implemented without undue complications, even for linear ones. Essentially, the degree of freedom of distributed parameter systems is infinite and the relevant mathematical theory is too complicated to be implemented in exergy analysis in HVAC applications. In principle, the distribution of exergy flow inside equipment can be investigated by combining exergy analysis and computational fluid dynamics (CFD)-based modelling. However, note that high-fidelity CFD simulations are very time-consuming and memory-intensive, especially for large-scale and complicated equipment. To overcome these limits, a reduced-order model (ROM) developed by integrating principal component analysis (PCA) with artificial neural networks (ANN) had shown a huge application potential to deal with the costly CFD-based simulation problem (Lang et al., 2011). The PCA-based ROMs for the nitrogen shock tube simulations (Bellemans et al., 2018) and the chemical reacting flows (Isaac et al., 2014) were also investigated, which had shown a great advantage of improving efficiency and accuracy. As for the multi-scale applications, a systematic ROM (Zhu et al., 2018) or the bi-level reduced modes (data-driven and physics-based) (Zhu et al., 2020) for CWCTs were developed by closely approximating the high-fidelity CWCTs models through utilizing HDMR or combined PCA-Kriging interpolation, which were further embedded in a multiscale optimisation model for performing integrated design and management of the CWCTs and cooling water system.

This paper presents an integrated framework that combines PCA and ANN methods for building bi-level ROMs for the heat and mass transfer processes in CWCTs. Due to the difference of characteristics between output variables and state variables, the ROMs for these two kinds of variables are constructed separately, which are referred to as yROM and zROM. With the developed framework, the exergy efficiency ratio based on yROM can be used for stochastic optimisation of exergy utilization, while the constructed exergy flux fields based on zROM provides a fast way for investigation of distributed exergy parameters in the flow field of CWCTs.

2. Exergy efficiency ratio and exergy flux field

In an HVAC system, the flow exergy of inlet air represents the maximum useful work done by air when it gradually saturated and approaches an equilibrium state relative to the dead state. Generally, exergy can be broken down into three components: thermal, mechanical, and chemical, as defined by Eqs(1-3).

$$ex_{a,them} = (C_{p,a} + \omega_a C_{p,v})\left[T_a - T_0 - T_0 \ln\left(T_a / T_0\right)\right] \tag{1}$$

$$ex_{a,mech} = \mathrm{R}T_0\left(1+1.608\omega_a\right)\ln\left(P_a / P_0\right) \tag{2}$$

$$ex_{a,chem} = \mathrm{R}T_0\left\{\left(1+1.608\omega_a\right)\ln\left[\left(1+1.608\omega_0\right)/\left(1+1.608\omega_a\right)\right]+1.608\omega_a\ln\left(\omega_a / \omega_0\right)\right\} \tag{3}$$

Multiplying the flow exergy by the mass flow rate gives the exergy flow rate, which can be expressed as follows:

$$\dot{Ex}_{a,i} = ex_{a,i} \times \dot{m}_a, \qquad i = \{them,\ mech,\ chem\} \tag{4}$$

where $C_{P,a}$ and $C_{P,v}$ are the specific heat capacities of dry air and water vapour; R is the gas constant; T_a, P_a, and ω_a are the temperature, pressure, and humidity of the inlet air; the subscript “0” and “a” represent the dead state and the air. In this work, the reference state at ambient temperature with saturated humidity ratio is selected as the dead state (Ren et al., 2002)

For the circulating water, only the thermal exergy is taken into account in exergy analysis since it is much larger than both the mechanical exergy and chemical exergy, as given in Eq(5). Besides, the total exergy flow rate of spray water introduced to the cooling tower is originally derived from the energy consumption of the spray pump, it can be given in Eq(6)

$$\dot{Ex}_{cw} \approx \dot{m}_{cw} C_{p.cw}\left[T_{cw} - T_0 - T_0 ln\left(T_{cw} / T_0\right)\right] \tag{5}$$

$$\dot{Ex}_{sw} = \dot{Q}_p = \dot{m}_{sw}\, gh / \eta_p \tag{6}$$

where $C_{p,cw}$ is the specific heat capacity of circulating water; T_{cw} and T_0 are the circulating water temperature and atmospheric temperature; g, h, and η_p are the gravitational acceleration, differential head, and mechanical efficiency; m and Q are the mass flow rate and energy consumption; the subscripts “cw”, “sw”, and “p” represent circulating water, spray water, and pump.

Exergy efficiency ratio. As defined in Eq(7), the exergy efficiency ratio is used as an optimisation index to evaluate the effective utilization of the purchased available energy. In this equation, the productive exergy is the exergy produced by heat transfer of circulating water, and the supplied exergy is the purchased exergy required to maintain the thermal system.

$$\eta = (productive\ exergy) / (supplied\ exergy) = \left(\dot{Ex}_{cw,in} - \dot{Ex}_{cw,out} \right) / \left(\dot{Ex}_{a,in} + \dot{Ex}_{cw,in} + \dot{Ex}_{sw,in} \right) \quad (7)$$

where $Ex_{cw,in}$, $Ex_{a,in}$, $Ex_{sw,in}$ stand for the exergy flow rates of input circulating water, humid air, and spray water; $Ex_{cw,out}$ stands for the exergy flow rate of output circulating water.

Exergy flux field. For an infinitesimal heat and mass transfer process, similar to "heat flux", a new concept of "exergy flux (W/m^2)" is used to explore flow exergy distributed on a control surface. As defined in Eq(8), it is a product of flow exergy and mass flux (j_a), which can be regarded as the flow exergy of a specific flowing fluid per unit of area per unit of time. Accordingly, the exergy flux fields include three types of distributed exergy fluxes such as thermal, mechanical, and chemical ones.

$$\dot{Ef}_{a,i} = ex_{a,i} j_a, \qquad i = \{them, mech, chem\} \quad (8)$$

3. Framework of building bi-level reduced-order models

For a given coupled heat and mass transfer system, the construction of its ROMs generally considers two levels of statistical data as follows: (1) lumped parameters related to the input and output streams, which are referred to as input variables ***X*** and output variables ***Y***; (2) distributed physical parameters in the multidimensional state space of interest such as temperature field, which is referred to as state variables ***Z***. Note that, both state variables and output variables should be mapped to its input variables for constructing a complete bi-level ROMs. Due to the difference of characteristics between output variables and state variables, the ROMs for these two kinds of variables should be constructed separately, which are defined as yROM and zROM. An integrated framework that combines PCA and ANN methods for building the ROMs is proposed in this work. It includes two steps including the experimental design and multi-sample CFD simulation, as well as the bi-level reduced-order modelling. More details about this integrated framework are as follows.

Determine a domain in the input space such as boundary conditions and CFD-related operating parameters.

(1) Implement a space-filling experimental design with SROM (Grigoriu, 2010) for input variables, to obtain a set of samples (**X**) within the input domain.
(2) Solve the CFD cases one-by-one with the obtained samples under the defined mesh by using CFD simulator. Then, we can obtain the values of the state variables and the output variables of interest such as exergy flux field (**Z**) and exergy efficiency ratio (**Y**), from the information stored in the CFD solutions.
(3) For yROM, with obtained **Y** and given **X**, implement the mapping **X**→**Y** by using ANN and then derive yROM: $x \rightarrow y = ANN_1(x)$.
(4) For zROM, with the selected reduced rank, PCA is performed for dimension reduction of obtained **Z** and the ranked principal components (PC) **W** and PCA score **Ψ** are obtained.
(5) Build the mapping **X** → **Ψ** by using ANN, and then formulate zROM: $x \rightarrow z = \mathbf{W}^{\mathbf{T}} \cdot ANN_2(x)$.

In step (4), the direct mapping from **X** to **Y** can be performed with ANN for the construction of yROM, but **Z** is a high dimensional snapshot dataset that is not suitable to map directly from **X**. PCA is used for dimension reduction on **Z** before constructing zROM. Because the magnitude of the considered variables is significantly different, the centering and scaling of the state values are necessary to increase the accuracy of the method. After the pre-processed operation, using the orthogonal decomposition, $\mathbf{Z} \in \mathbb{R}^{p\times N}$ with N samples of q original variables is then decomposed via $Z = W^T\psi + \varepsilon$. In this way, the matrix **Z** is decomposed into PCA scores $\mathbf{\Psi}=[\Psi_1, \Psi_2, \ldots, \Psi_\alpha]^T \in \mathbb{R}^{\alpha\times N}$ and PC matrix $\mathbf{W}=[W_1, W_2, \ldots, W_\alpha]^T \in \mathbb{R}^{\alpha\times p}$, N and p represent the number of simulations and the number of grids. The number of PCs α is referred to as a reduced rank, which is the representation dimension of **Z** after PCA, while **ε** represents an error caused by dimension reduction. W_i, i=1…α, in the **W** sorted in descending order of importance, is the eigenvector of $\mathbf{ZZ}^T$, which represents a specific PC of the **Z**, and each PC has an associated eigenvalue, λ_i, it represents the variance of the original data taken into account by that PC. The greater λ_i is, the more data information is contained in the corresponding PC W_i. The high-dimensional **Z** of observed state variable can be encoded into a lower-dimensional **Ψ**, and **Ψ** can relate to **Z** based on the first few PCs with negligible error, then we can implement mapping from **X** to **Ψ** instead directly to **Z**.

4. Results and Discussion

The schematic structure of CWCT and the coil zone investigated in CFD simulation are shown in Figure 1. In this work, COMSOL Multiphysics is used to simulate three-dimensional steady-state CWCT. The mass flow rate and pressure outlet boundary conditions are imposed on the inlet and outlet of the air and circulating water, while the heat source and moisture source is utilized to model the evaporation of spray water. The detailed description and validation of the CFD model can be found in our previous study (Xie et al., 2019). Note that, in the direction of *x-z* axes (Figure 1b), only two complete and two halves tubes are simulated due to the symmetry principle. The input variables for the CWCT operation comprises of uncertain variables and control variables as reported in Table 1. As aforementioned, SROMPy (Warner, 2018) is used to generate 100 design points from the input space, resulting in a stochastic sample set $\mathbf{X}\in\mathbb{R}^{100\times4}$. Consequently, the sample set is used as model inputs for the multi-sample CFD simulations. After convergence, the results of both the output variables related to streams and the state variables in the fluid field are recorded. These two types of recorded results, together with the input variables are used to construct yROM and zROM by using Matlab, as detailed in Section 3.

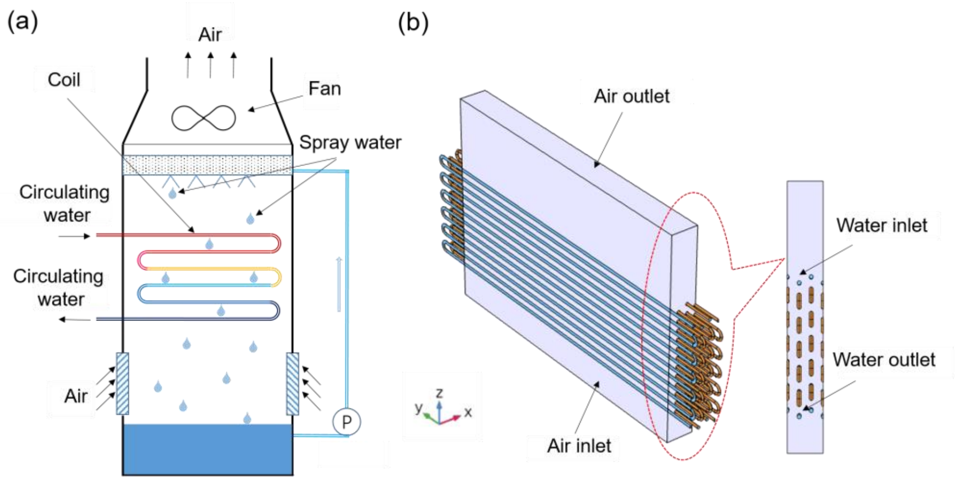

Figure 1: (a) The structural representation of CWCT; (b) the control volume and cross-section of the coil zone

Table 1: Input space and parameter specification

Input space	Symbol	Unit	Specification
Control variables			
volumetric flow rate of inlet air	q_a	m^3/s	U(1.0, 3.0)
mass flow rate of spray water	q_{sw}	kg/s	U(1.0, 2.0)
Uncertain variables			
dry bulb temperature of inlet air	T_0	^oC	nonparametric distribution
relative humidity of inlet air	ω_0	-	nonparametric distribution

To maximise the exergy efficiency ratio of the system under uncertainty, the constructed yROM is incorporated into a stochastic optimisation model through Matlab. In this optimisation model, the objective is maximising the exergy efficiency ratio, and the control variables are decision variables and need to be optimized at specified ranges, while the uncertain variables are specified to the values and probabilities according to sampled points. To meet the requirements of the cooling targets, the outlet temperature of the circulating water should be equal to or lower than a specified value. The optimal solutions denoted by green dots at different air dry-bulb temperatures are shown in Figure 2. Note that, field-based the original results based on randomly sampled operating points are also provided in this figure. As shown, compared with the original results without optimisation, the optimal flow rates of the inlet air have a remarkable increase, some of them even have reached the upper bound. On the contrary, for all sample points, the optimal flow rates of the spray water are significantly reduced to the lower bounds after optimisation. In summary, the increase in air flow rate and the decrease in the spray water flow rate can improve the exergy efficiency ratio of the investigated CWCT.

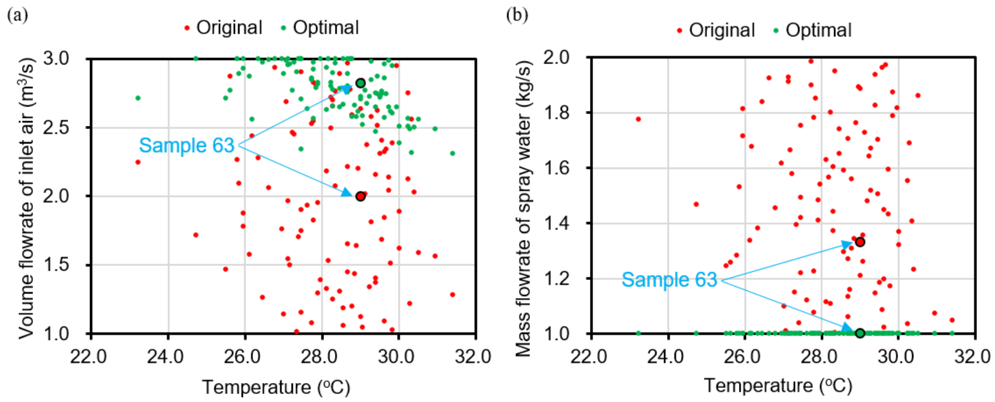

Figure 2: The results of stochastic optimisation with trained yROM

The Sample 63 is selected for illustrating and analysing the influence of stochastic optimisation on the exergy flux fields. By using the constructed zROM, the filled contours of thermal-, mechanical- and chemical- exergy flux fields are all reconstructed and shown in Figure 3. For each contour, the variation of exergy fluxes after optimisation gradually becomes obvious from down to the top of the tower with upward airflow, particularly in the upper coil rows. In Figure 3a, the thermal exergy flux slowly increases at the top of the coil zone because the heat transfer from circulating water increases the temperature of upward air. However, note that the interaction between upward air and downward spray water in the coil zone not only decreases the hydraulic pressure of air but also increases the relative humidity due to mass transfer. This leads to the destruction of mechanical and chemical exergy. In Figure 3b,c, both the mechanical and chemical exergy fluxes have significant decrements in the entire coil zone.

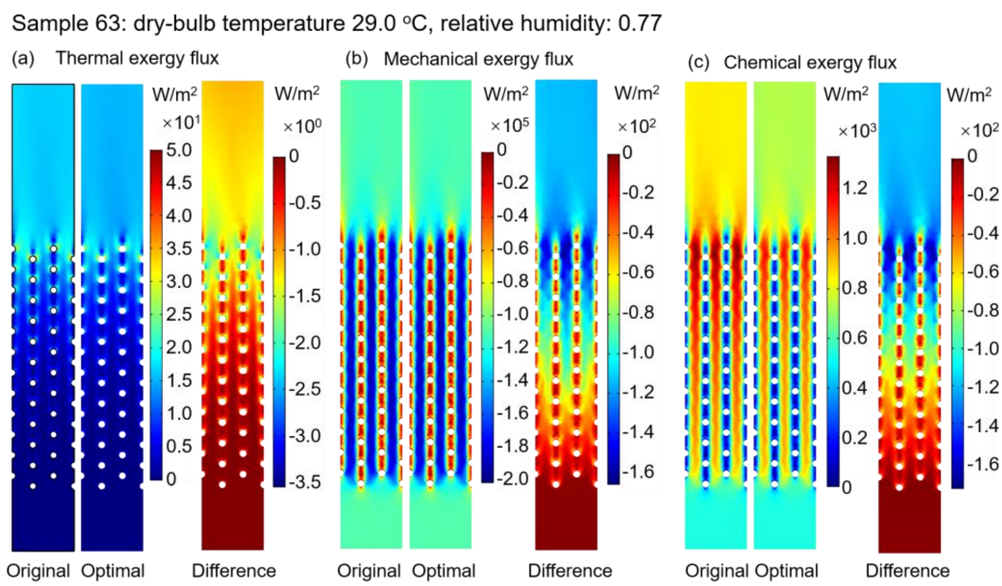

Figure 3: Comparison of exergy flux fields based on the original and optimal solutions of Sample 63

By comparing the original and optimal images, it can be seen that the profiles of the three exergy flux fields have nearly the same distributions, in particular for the thermal- and mechanical- exergy flux fields. The difference of contours between optimal and original solutions indicates that the three exergy fluxes on average decreases after optimisation. The decreased values of the mechanical and chemical exergy fluxes range from 0~160 W/m^2, which are significantly greater than that of the thermal exergy flux ranging from 0~3.5 W/m^2. This phenomenon clearly reflects that the performance improvement on the exergy efficiency ratio mainly results from the reductions of mechanical and chemical exergies. Finally, it should be noted that the CPU time is significantly reduced from several hours or more for CFD simulation to a few seconds for the ROM evaluation, which further makes the iterative optimisation tasks realizable.

5. Conclusions

In this work, an integrated framework based on model-reduction that combined PCA and ANN methods was proposed for building a bi-level ROMs. It mainly followed two steps that include the experimental design and multi-sample CFD simulation, as well as the bi-level reduced-order modelling. The developed yROM based on the exergy efficiency ratio for CWCT was used for stochastic optimisation, while the exergy flux field-based zROM was utilized for analysing the distributed exergy parameters inside the equipment. The optimisation results showed that the increase in air flow rate and decrease in spray water flow rate can improve the exergy efficiency ratio of the CWCT. The thermal exergy flux slowly increased at the top of the coil zone, while both the mechanical and chemical exergy fluxes had significant decrements in the entire coil zone. The decreased values of the mechanical and chemical exergy fluxes ranged from 0~160 W/m^2, which were significantly greater than that of the thermal exergy flux ranging from 0~3.5 W/m^2.

Though the case studies showed that the proposed bi-level ROM methodology was both effective and efficient for the presented study. Yet, many limitations still existed, e.g., how to define the hyper-parameters; how to reduce the sizes of sampled points, the hidden layers in the ANN, and the retained PCs, etc. These influencing factors should better take into account in the future study to improve the accuracy of the ROM.

Acknowledgements

Financial support from the National Natural Science Foundation of China (51776228) is acknowledged.

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