SENSITIVITY ANALYSIS AND IDENTIFICATION
OF AN EFFECTIVE HEAT TRANSPORT MODEL IN WAVY LIQUID FILMS

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ABSTRACT
Thin liquid films flowing down vertical or inclined planes are of high industrial relevance. Nevertheless, a predictive transport model describing the effects of wave-induced intensification of heat and mass transport for the design of technical systems does not yet exist. In this paper, a systematic approach for the identification of a suitable transport model (structure and parameters) for the effective heat transport coefficient in the reduced system of heat transport equations is presented. For this transport coefficient, two different model structures are proposed. An investigation of parameter identifiability based on local sensitivity analysis is carried out for both model structures prior to model identification. It is shown that the number of model parameters can be significantly reduced by targeted selection of the identifiable parameter subsets. This facilitates to reduce the overall computational effort. After setting up the best identifiable parameter sets for each model structure, a nonlinear, constrained least-squares parameter estimation problem is stated and solved using standard solution methods. Automatic differentiation techniques are applied for efficient sensitivity computations as well as for the gradients calculation within the parameter estimation step. Finally, the best model candidate is determined using statistical model discrimination techniques.

NOMENCLATURE

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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<tbody>
<tr>
<td>J</td>
<td>Objective functional</td>
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<tr>
<td>σ</td>
<td>Standard deviation</td>
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<tr>
<td>θ</td>
<td>Vector of parameters</td>
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<tr>
<td>S</td>
<td>Sensitivity matrix</td>
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<td>V</td>
<td>Covariance matrix</td>
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<tr>
<td>R</td>
<td>Correlation matrix</td>
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<td>γ</td>
<td>Collinearity index</td>
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INTRODUCTION
Thin liquid films flowing down vertical or inclined planes have been the subject of intensive research particularly because of their industrial relevance. Despite this considerable research effort, the dynamics of nonlinear waves typically present in such flows and their effects on scalar transport is still not satisfactorily understood. As a direct CFD simulation of film flows is computationally expensive, a simple predictive model describing the effects of wave-induced intensification of heat and mass transport would greatly contribute to the design of technical systems. Such a model is not yet available. One approach to reduce the complexity of the transport equations in the film flow consists of introducing the effective transport coefficients to describe the enhancement of the transport processes [1].

The most challenging task is the development and identification of a suitable model for these transport coefficients which is widely applicable and of sufficient predictive quality. The model structure has to be inferred from experimental data employing reasonable assumptions and available theories. In most of the cases, several competing candidate model structures may be proposed. In order to obtain the best model, the parameters of each of the available candidates have to be estimated. Model discrimination techniques have to be applied to choose the best model on the basis of some
reasonable measure of model validity [2]. Yet, such a parameter estimation problem involves optimization methods dealing with the transport equations and their derivatives, which are, even for a relatively low number of model parameters, numerically hard to handle and computationally expensive. Moreover, the estimation may lead to a biased estimate or may even fail if the underlying model is over-parameterized or the model structure is incorrect [3, 4]. Therefore, a systematic a priori approach is necessary to assess model suitability and parameter identifiability from available experimental data prior to parameter estimation [4].

In the present work, a heat transport model based on the concept of effective transport coefficients is developed. Moreover, a systematic approach for its identification is proposed. The quality of the obtained model is investigated based on experimentally validated simulated temperature data stemming from two-dimensional, transient numerical simulation of the heat transfer in a stable wavy film [5, 6]. We address two model structures for the effective thermal diffusivity in the simplified system of transport equations, one with a low number (two), and a second with high number (eight) of parameters. We adopt this last model from [6], where it has been identified using the error-equation method [7]. For each model structure the problem of parameter identifiability from available simulation data is investigated using sensitivities of the data w.r.t. model parameters. In this way the identifiable parameter subsets are determined for each model candidate after which the parameters are estimated by solving the constraint least-squares estimation problem using standard solution methods [8]. The sensitivities and gradients thereby are computed using automatic differentiation techniques [9, 17]. Subsequently, the best model is identified by discriminating between originated candidate models [10].

The paper is organized as follows. First, we present the heat transport model with effective thermal diffusivity. Then, the systematic identification procedure together with sensitivity-based tools and criteria for a priori parameter identifiability analysis are outlined. The employed automatic differentiation strategy for the calculation of derivatives is briefly introduced. The results obtained are discussed and finally, conclusions are given.

**EFFECTIVE HEAT TRANSPORT MODEL**

The major reason for the high computational cost of direct transient numerical simulation of wavy film flow is due to the multiphase character. In order to reduce the problem complexity, the two-dimensional time-varying domain corresponding to the liquid phase is mapped to a two-dimensional time-invariant waveless domain. In this way, a two-phase transient problem reduces to a single-phase steady-state problem. The system of governing equations has to determine the temperature and velocity fields mapped from the real wavy to the modelled flat film domain. As a substitute, an effective thermal diffusivity model is introduced [1] to capture all wave-induced heat transport effects in the reduced flat film geometry.
effective diffusion coefficients. For this purpose, we use the general formulations
\[ a_{\text{eff}}(T, \theta') = f(T, \theta'), \quad a_{\text{eff}}(T, \theta') = g(T, \theta'), \]  
where \( \theta' \in \mathbb{R}^n, \theta' \in \mathbb{R}^n \) denote unknown parameters and \( f(\cdot) \) and \( g(\cdot) \) represent reasonable model structures. To simplify the presentation, we combine these unknown parameter vectors in one large column vector as
\[ \theta = [\theta^T, \theta^T] = [\theta_1, \ldots, \theta_p]^T, \quad p = n + m. \]  
By inserting the transport model (2) into the energy balance (1), the non-linear system of heat transport equations is obtained
\[ u_{\text{nf}} \frac{\partial T}{\partial y} = \frac{\partial}{\partial x} \left( f(T, \theta') \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left( g(T, \theta') \frac{\partial T}{\partial y} \right), \]  
with following boundary conditions (cf. Fig. 1)
\[ T|_{y=0} = T_0, \quad T|_{y=L} = T_w, \quad \frac{\partial T}{\partial y}|_{y=0} = 0, \quad \frac{\partial T}{\partial y}|_{y=L} = 0. \]  
\( T_0 \) and \( T_w \) denote the constant temperatures at the inlet \( (x=0) \) and wall \( (y=0) \) boundaries. At the outlet \( (x=L) \) and the fluid interface \( (y=\delta_w) \) zero diffusive flux conditions are considered.

**SYSTEMATIC IDENTIFICATION APPROACH**

The model identification procedure for the transport coefficients follows four steps:

(i). Select candidate models.

(ii). Perform parameter identifiability analysis and identify identifiable parameter subsets.

(iii). Estimate identifiable parameters.

(iv). Discriminate between alternative models.

Note that step (ii) in this scheme is especially advantageous, since unsuccessful parameter estimation runs are avoided, because only identifiable parameters are estimated for each model candidate. This significantly saves the overall computational and engineering effort.

As noted before, based on different assumptions and theories competing model structures of the effective thermal diffusivities can be proposed. In step (iv), the best model has to be determined using some model discrimination techniques. In this paper we apply the well-known Akaike information criterion [10]. This criterion seeks a compromise between model fit and number of model parameters.

The estimation problem (step (iii)) represents a so-called *simultaneous* problem, since all assumptions made w.r.t. model structure (cf. (2)) will simultaneously influence the identification. Such models lead to biased or poor estimates, in case the model structure is incorrect [3]. Satisfactory results can typically be achieved if the correct model structure is known. Therefore, it is of crucial importance to carry out the identifiability analysis (step (ii)), to determine the influences of the model and parameter uncertainties. In this way, the possible problems arising in the parameter estimation step, like e.g. the divergence of the optimization algorithm, can be largely reduced or even avoided [4, 12].

**PARAMETER ESTIMATION**

The parameter estimation problem can be formulated in a generic way as follows. Let \( N \) be the number of temperature measurements \( \tilde{T}(Y_\mu), \mu = 1, \ldots, N \) at spatial coordinates \( Y_\mu \in \Omega \) with additive normally distributed measurement error \( \varepsilon \) of zero mean and constant variance \( \sigma^2 \), i.e.,
\[ \tilde{T}(Y_\mu) = T(Y_\mu; \theta) + \varepsilon_\mu, \quad \mu = 1, \ldots, N, \]  
where, \( T(Y_\mu; \theta) \) denotes the temperature predicted by the transport model (4) for some prescribed values of the parameters projected on the spatial coordinates \( Y_\mu \). To obtain optimal estimate \( \theta' \), we minimize the nonlinear least-squares objective function
\[ J(\theta) = \sum_{\mu=1}^{N} \frac{(T(Y_\mu; \theta) - \tilde{T}(Y_\mu))^2}{2\sigma^2}, \]  
subject to the model (4), to suitable Ansatz functions for \( f(\cdot) \) and \( g(\cdot) \), and constraints
\[ f(T, \theta') > \eta > 0, \quad g(T, \theta') > \zeta > 0, \]  
where the constants \( \eta \) and \( \zeta \) stem from the ellipticity condition of the equation system (4) [13].

The efficient solution of the estimation problem (6) involves gradients of the transport model (4) w.r.t. parameters \( \theta \in \mathbb{R}^p \). Therefore, even for a low number of parameters, it is computationally expensive, such that a careful analysis prior to its actual solution is appropriate.

The accuracy of the parameter estimates is measured by their covariance matrix. In the case of the available initial guess \( \theta^0 \in \mathbb{R}^p \) for the parameters, an a priori estimate of the covariance matrix \( V \in \mathbb{R}^{p\times p} \) can be calculated [14]. Its entries are given by
\[ v_{ij} = \sigma^2 \left( \sum_{\mu=1}^{N} y_{\mu} \psi_{\mu} \psi_{\mu}^T \right)^{-1}, \quad i, j = 1, \ldots, p \]  
(7)

where

\[ \psi_{\mu} = \frac{\partial T(Y; \theta^0)}{\partial \theta_j}, \quad \mu = 1, \ldots, N, k = 1, \ldots, p \]  
(7a)

The matrix \( V \) gives a lower bound on the uncertainty to be expected for the parameter values. Note that, this estimate is exact only for linear models. Its use for the nonlinear models seems, however, to be quantitatively quite acceptable [14]. Given \( V \), the (approximate) standard deviation of the \( i \)-th parameter \( \theta_i \) can be evaluated as

\[ \sigma_i = \sqrt{v_{ii}}. \]  
(8)

In addition, the confidence ellipsoids can be computed [14]. The smaller the value \( \sigma_i \), the better is the confidence in the parameter \( \theta_i \).

The computation of the covariance matrix (7) requires knowledge of the measurement error variance \( \sigma^2 \). In this paper, the Gasser, Sroka & Jennen-Steinmetz (GSJ) estimator [15] is used for its estimation, because it is known to be simple and robust [12].

PARAMETER IDENTIFIABILITY

In this section, we introduce tools and criteria for quantitative assessment of a parameter estimation problem prior to its solution. Thereby, we want to provide the criteria ensuring the identifiability of the parameters \( \theta \in R^p \) from the available data. For the purpose of this analysis, the model structures for the effective thermal diffusivities (cf. (2)) are kept fixed, while the parameters are adjusted to fit the data.

In order to assess parameter identifiability from available (experimental or simulation) data, however, the effects of the joint influence of the parameters on the model output have to be considered, that is, the interdependency of the parameters should be quantified. This is accomplished by construction of the correlation matrix \( R \in R^{p \times p} \) with entries

\[ r_{ij} = \frac{v_{ij}}{\sqrt{v_{ii} v_{jj}}}, \quad r_{ii} = 1, \quad i, j = 1, \ldots, p. \]  
(9)

Large off-diagonal absolute values of the elements in the correlation matrix indicate a strong dependency of parameter estimates. In other words, different parameter values can lead nearly to the same model output, hence the involved parameters are poorly identifiable [4]. Yet, the correlation matrix for a subset of \( k \) parameters \( (2 < k \leq p) \), does not reveal correct information about the pairwise parameter dependencies, because the parameters with significant bias sources are still not explicitly fixed.

To further tackle the parameter dependency in a more rigorous manner, the collinearity index is used [4]. The collinearity index is based on the scaled sensitivity matrix \( S \in R^{k \times p} \) with entries given as

\[ s_{\mu j} = \frac{\partial T(Y; \theta^0)}{\partial \theta_j} \frac{\Delta \theta_j}{SC_\mu}, \quad \mu = 1, \ldots, N, j = 1, \ldots, p \]  
(10)

where \( \Delta \theta_j \) is a priori measure of the reasonable range of \( \theta_j \), and \( SC_\mu \) is a scale factor with the same physical dimension as the \( \mu \)-th measurement. To assess the degree of parameter dependencies in a subset of \( k \) parameters \( (1 \leq k \leq p) \), first, the normalized sensitivity matrix \( \tilde{S} \in R^{k \times p} \) is defined with the columns given as

\[ \tilde{s}_j = s_j, \quad j = 1, \ldots, p. \]  
(11)

\( s_j \) denote here the columns of the sensitivity matrix \( S \). The collinearity index \( \gamma_k \) is then given as

\[ \gamma_k = \frac{1}{\sqrt{\lambda_k}}, \]  
(12)

with \( \lambda_k \) the smallest eigenvalue of \( \tilde{S}_k \tilde{S}_k^T \), whereas the matrix \( \tilde{S}_k \) contains the columns of \( \tilde{S} \) that correspond to the parameters in a subset \( K \). The larger \( \gamma_k \), the higher the dependency between the parameters. Or in other words, a change in one parameter \( \theta_j \in K \) can be compensated up to a fraction of 1 divided by the collinearity index \( \gamma_k \) by appropriate changes in the other parameters in \( K \).

From a practical point of view, a collinearity index of 20 means that a change of the calculated results caused by a tuning of a one parameter in \( K \) can be compensated to the average of 5% by appropriate changes in the other parameters in \( K \) [4]. A high value of the collinearity index thus indicates poor identifiability of the parameter set \( K \). To identify suitable parameter sets we consider the range of 5-20 as threshold values for \( \gamma_k \) (see [4] for details). Note that, \( \gamma_k \) does not depend on the choice of the \( \Delta \theta_j \), because of normalization of \( S \). However, it is sensitive to the choice of the scale factors \( SC_\mu \) and naturally, it depends on \( \theta^0 \).
TRANSPORT MODEL SENSITIVITIES

The main ingredient of the a priori identifiability analysis is the computation of the sensitivities (7a). Given these, the construction of the covariance (cf. (7)), correlation (cf. (9)) and scaled sensitivity matrices (cf. (10)) is straightforward. Apart from sensitivities, the gradient of the objective functional (6) w.r.t. parameters is required within the optimization step. These two core components are obtained using automatic differentiation.

In the forward problem (4) the temperature $T$ for prescribed values of the parameters $\Theta \in \mathbb{R}^p$ results from executing a simulation code. A straightforward approximation to the sensitivities (7a) can therefore easily be implemented by numerical differentiation using divided differences, i.e. by calling this computer program multiple times with suitable perturbations of the input parameters $\Theta$. In certain cases, suitable perturbations are known in advance. In general, however, it can become notoriously difficult to find perturbations leading to meaningful derivatives. The reason is that, on the one hand, the perturbations should be small minimizing the truncation error of the divided differences and, on the other hand, the perturbations can not be too small to avoid excessive cancellation error in finite-precision arithmetic. Therefore, we rely on truncation-error free techniques based on automatic differentiation. In this set of techniques, a given computer program is mechanically transformed into a new computer program for the computation of user-specified derivatives. In this paper, the recent automatic differentiation tool ADiMat [16] is used to transform the forward solver into a new program capable of computing the sensitivities (7a). More details on automatic differentiation are available on www.autodiff.org and in [9, 17].

NUMERICAL RESULTS

In this section the proposed model identification scheme is applied to the system of heat transport equations (4) by posing two different pairs for transport models $f_i(\cdot)$ and $g_i(\cdot), i = 1, 2$, for effective thermal diffusivities $\alpha_{\text{eff}}^i$ and $\alpha_{\text{eff}}^j$ (cf. (2)). The study is carried out using simulated temperature data $\tilde{T}_{\text{sim}}$ stemming from the two-dimensional, transient numerical simulation of energy transport in a stable wavy film flow. The simulation was performed by the commercial CFD package FLUENT and was validated by experimental data [5]. It was carried out for different values of Reynolds and Prandtl numbers at a constant wave excitation frequency [6]. The duration of the simulation was adjusted to obtain thermally fully developed flow. In this paper we restrict the presentation of the case study to $Re = 20$ and $Pr = 56$. A kinematic viscosity of the fluid was $\nu = 4.7 \cdot 10^{-5} [m^2/s]$ at an inlet temperature $T_0 = 300[K]$. The corresponding value of the Nusselt film thickness and the Nusselt velocity are $\delta_{Nu} = 5.13 \cdot 10^{-4} [m]$ and $u_{Nu} = 0.27 \cdot \left( 2 \cdot y / \delta_{Nu} - \left( y / \delta_{Nu} \right)^2 \right)$, respectively. In the calculations, $L = 0.18 [m]$ was set and the wall temperature was kept constant at $T_w = 350[K]$.

The temperature data obtained from the simulation of the wavy film $\tilde{T}_{\text{sim}}$ were mapped to the model domain by spatial transformation and subsequent time averaging. Details are given in [6]. We denote the transformed data by $T_{\text{sim}}$. In our case, the spatial transformation was carried out on a grid of 25 points in flow and 106 points in perpendicular direction, whereas time averaging over one period length in the thermally developed state of the film flow was performed.

Two model structures are considered. In the first scenario (referred to in the following as scenario I), we assume constants for both $\alpha_{\text{eff}}^i$ and $\alpha_{\text{eff}}^j$ in (2), i.e.,

$$f_i(\Theta^*) = \theta_1 \quad \text{and} \quad g_i(\Theta^*) = \theta_2. \quad (13)$$

As a second scenario (referred to in the following as scenario II), the parametric model with 8 parameters introduced in [6] is used, i.e.

$$g_2(\Theta^*) = \alpha_{\text{mod}} \cdot \nu / \text{Pr} = \text{const}.$$  

$$g_2(\Theta^*) = \alpha_{\text{mod}} + 1000 \sum_{i=1}^6 \theta_i \chi^{(n-1)} \left( y^* \right) \chi^2 \left( y^*, \theta_2, \theta_7 \right) \quad (15)$$

$\alpha_{\text{mod}}$ denotes the known constant molecular thermal diffusivity of the fluid. Hence, in the flow direction pure molecular diffusive heat transport is assumed. In perpendicular direction, however, the wave induced effects are modelled. The dependence of $\alpha_{\text{eff}}^j$ on $x^* = x / L$ (cf. Fig. 1) is expressed by a polynomial of 5$^{th}$ order, while the dependence on $y^* = y / \delta_{Nu}$ is a Chi-Squared type function with $\theta_7$, being the number of degrees of freedom and $\theta_7$ the scaling factor.
To estimate parameters in each of the two scenarios, the least-squares problem (6) must be solved. For this purpose, a forward numerical solver of equations (4) was implemented in MATLAB. An upwind scheme was used for discretization and the GMRES method [18] was employed for the solution of the discretized equation system. The same discretization of 25×106 points used in the spatial transformation of the simulated temperature data was employed to discretize the system of equations (4). For the calculation of gradients for optimization and of the sensitivities for sensitivity analysis, the forward solver was transformed into a new program using ADiMat [16]. For optimization, the MATLAB-implemented internal software was used, which offers an easy-to-implement, user-friendly programming environment for applying different solution algorithms to the problem at hand. SNOPT [8] is used for the solution of the considered nonlinear optimization problem.

Scenario I: For the two-parameter scenario, the initial guess \( \theta^0 = (\alpha_{mol}, \alpha_{mol}) \) is considered and the covariance and correlation matrices (cf. (7), (9)) are computed. From the confidence ellipsoid for this scenario, it can be seen that the standard deviation of \( \theta \) is of significant magnitude. The off-diagonal entries of the correlation matrix are \( r_{12} = r_{21} = 0.61 \), whereas the collinearity index for full parameter set results in \( \gamma_{\{1,2\}} = 1.59 \). This reveals, that the two parameters are largely uncorrelated.

In Fig. 3 the estimation result after 4 major optimization iterations, corresponding to the optimal value of
\[
\theta^* = (12.01, 1 \cdot 10^{-4})
\]
(16) is presented. Because of the non-linearity of the objective functional (6a), the solution of the optimization problem (6) is very sensitive to the choice of feasible set (cf. (6b)). The results presented correspond to the values of \( \eta = \zeta = 10^{-4} \). Smaller values lead to local solutions of a very low quality. We observe good model agreement on a large region as shown in Fig. 3 (b), but also locally large estimation errors. Thus, the model (13) cannot recover the whole behaviour observed in the data, as could be expected from the very simple model structure in this case. The obtained parameter values (16) show also that the effective diffusion in flow direction largely dominates the other one.

Scenario II: As an initial guess in the 8 parameter scenario (15), the following optimal estimation from [6]
\[
\theta^0 = (-0.0013, -0.07, 1.42, -3.93, 4.05, -1.45, 3.34, 4.34)^T
\]
(17) is used. This value corresponds, however, to the dynamical thermo-fluid state of the flow. Nevertheless, it is a good initial approximation for performing an a priori analysis and the subsequent estimation step.

Using this initial value the covariance and correlation matrices are computed. The standard deviations for each parameter is (in percent)
\[
(\sigma_{\alpha,\min}, \sigma_{\min}) = (3.36, 2.7, 2.23, 2.07, 5.14, 10.31, 1.07, 1.46),\]
which is large for some of the parameters. The correlation matrix is as well dominated by the entries with absolute value greater than 0.9. This indicates high correlation of several parameters. To filter out these highly correlated parameter subsets, the collinearity indices of all possible (255) subsets of the 8 parameters are computed. The collinearity index for the full parameter set resulted in \( \gamma_{\{1,..,8\}} = 1158 \), rendering all 8 parameters unidentifiable. In Tab. 1 the parameter sets having the lowest values of the collinearity index below the threshold of 20 are presented. This result reveals that the large parameter uncertainty presented in the full parameter set can be reduced by estimating a significantly lower number of parameters.

<table>
<thead>
<tr>
<th>dim</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
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<tr>
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<td>{1,6}</td>
<td>{1,4,7}</td>
<td>{1,6,7,8}</td>
<td>{1,3,6,7,8}</td>
</tr>
<tr>
<td>( \gamma_{K,\text{min}} )</td>
<td>1.31</td>
<td>1.86</td>
<td>4.26</td>
<td>11.56</td>
</tr>
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</table>
While doing so, all the remaining parameters are fixed to their initial values. Note that, the parameter subset \{1,6\} is redundant as it fixes all the parameters modeling wave induced effects in the model structure (15). Therefore, we omitted this subset from the estimation step. Note also, that in this scenario the optimization problem (6) is nonlinearly constrained (cf. (6b)). \(\zeta = 10^{-10}\) is used as a lower bound for \(g_1(\cdot)\) in (6b).

Despite the very high collinearity index \(\gamma_1 = 1158\) for the full parameter set, we included this set in the estimation step to gain an insight of possible problems with the optimization in such cases. The estimation result after 1 major optimization iteration corresponding to the optimal value

\[
\theta^* = (-0.24, 0.84, -0.96, 0.39, -0.02, -0.004, 3.59, 5.16)^T
\]  

(18)
is presented in Fig. 4. All parameter values have been changed by the optimization.

![Figure 4: Scenario II with full parameter set (a) temperature profiles at \(x = L/2[m]\) (cf. Fig. 1), (b) the deviation between the data and estimated temperatures](image)

It can be seen that the initial value is significantly improved, but that the deviation is still partially present (cf. Fig. 4(b)). It is important to note, that the good initial value facilitated the convergence of the solution, such that only 1 major optimization iteration was necessary. Convergence fails for the full parameter set in the case of bad initial values. This is due to the high correlation of the parameters. This leads to a large number of iterations in the optimization, since different combinations of the highly correlated parameters yield almost the same results. We observe also a systematic deviation in the estimation.

**Model discrimination:** We further estimated the remaining three reasonable parameter subsets \{1,4,7\}, \{1,6,7,8\}, \{1,3,6,7,8\} (cf. Tab. 1) within the model structure (15) while fixing the remaining non-estimated parameters at the initial values (17). Subsequently, discrimination of five models - (13), (15) with full parameter set and (15) with three reduced parameter subsets as above, was carried out applying the Akaike information criterion [10].

The model structure (15) with the parameters in subset \{1,4,7\} adjusted the remaining parameter values fixed at the corresponding initial values turned out to be as the best model. The corresponding values of the Akaike information criterion (\(AIC\)) are given in Tab. 2.

![Table 2: \(AIC\) values for the selected parameter sets](image)

<table>
<thead>
<tr>
<th>Subset</th>
<th>(AIC)</th>
<th>(\Delta AIC)</th>
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<tr>
<td>sc. I</td>
<td>{1,2}</td>
<td>-0.004, 3.59, 5.16</td>
</tr>
<tr>
<td>sc. II</td>
<td>{1,4,7}</td>
<td>1.36 \times 10^4</td>
</tr>
<tr>
<td>AIC</td>
<td>1.80 \times 10^4</td>
<td></td>
</tr>
<tr>
<td>AIC</td>
<td>1.24 \times 10^4</td>
<td></td>
</tr>
<tr>
<td>AIC</td>
<td>1.71 \times 10^4</td>
<td></td>
</tr>
<tr>
<td>AIC</td>
<td>1.22 \times 10^4</td>
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</tr>
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In Fig. 5, the estimation results using this model are presented. 4 major optimization iterations were required to obtain the optimal solution

\[
\theta^* = (0.012, -0.07, 1.42, -3.95, 4.05, -1.45, 0.53, 4.34)^T
\]  

(19)

![Figure 5: Scenario II with three parameter subset (a) temperature profiles at \(x = L/2[m]\) (cf. Fig. 1), (b) the deviation between the data and estimated temperatures](image)

Clearly, the values of parameters \(\theta_1\) and \(\theta_7\) have been significantly changed, such that a better fit of the data is achieved. The small value of the optimal parameter \(\theta_7\) indicates for the lower significance of the effective diffusion relative to that of molecular one (cf. [6] for more details), which is expected for relatively low Reynolds numbers. Looking at the results in Fig. 4 and 5, we observe, as in the previous scenario, a good agreement of the model on a region of the domain, but also larger estimation errors on the other parts. The error magnitude is much smaller than that in scenario I. This indicates that also the model structure (15) in this scenario II, cannot capture the whole system behavior and needs further improvement. This issue will be addressed in a future work.
CONCLUSIONS
An effective transport model has been studied and systematically identified using simulated CFD data. A major ingredient is that prior to the parameter estimation step, identifiable parameter subsets are determined. In this way, the number of parameters to be adjusted can be significantly reduced. Highly nonlinear simultaneous estimation problems with different models for the transport coefficient have been solved. The accomplished study shows that the model structures, although very simple, they recover some of the features of the heat transport. However, the results reveal also the necessity of an improved model structure, which is capable of precisely capturing the effects of effective transport as observed in the data. In the future work, we will use a model structure with few parameters in both flow and perpendicular directions to study the influence of the effective transport of film flow. Moreover, different flow conditions, i.e. different Reynolds and Prandtl numbers will be considered, to come up with a model of sufficient engineering applicability.

ACKNOWLEDGMENTS
The authors gratefully acknowledge the financial support of Deutsche Forschungsgemeinschaft (DFG) within the Collaborative Research Center (SFB) 540 “Model-based experimental analysis of kinetic phenomena in fluid multiphase reactive systems”. Special thanks go to Dr. Sven Groß for fruitful discussions and useful advices.

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