Incremental Identification of Transport Models in Falling Films

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ABSTRACT

In this paper, an incremental identification method is presented to systematically determine an effective transport coefficient model in the flat-film model of a falling film from high resolution measurements. While the convective velocity in the three-dimensional, transient convection-diffusion equation is known, the diffusion term is characterised by an unknown, transport coefficient to account for the neglected backmixing in the flat-film model. To efficiently treat the nonlinear and ill-posed inverse problem of transport coefficient model identification, the problem is decomposed into a sequence of easier to handle subproblems. This strategy aims at the determination of the best-performing transport coefficient model in a transparent decision-making process, in particular, in those cases where a-priori knowledge on the model structure is lacking. Yet, to result in an accurate model, a careful design of the experimental conditions has to be carried out. In this paper, an optimally designed falling film experiment for a three-dimensional flat-film model is designed for the first time to support the identification of a high precision transport coefficient model.

1 INTRODUCTION

Liquid falling films occur in many multiphase unit operations, such as packed columns, falling film reactors or evaporative cooling towers. Falling films show complex dynamics and nonlinearity due to developing surface waves [1], which intensify transport phenomena [2]. Despite the considerable research effort spent, the intensification mechanisms are still not well understood and detailed transport models to support equipment design are still lacking.

The complex fluid dynamics of the free liquid phase boundary renders a direct numerical solution (DNS) of the film model in three space dimensions numerically challenging and computationally demanding. Hence, DNS can not be employed for equipment design. Therefore, the transport model has to be simplified such that the intensification of the transport processes can still be predicted with sufficient accuracy. In this simplified model, the real, free boundary problem is approximated by a three-dimensional transport problem with rectangular geometry and known, stationary boundaries (cf. Figure 1, [3]). Effective transport coefficients are introduced in this flat-film model to capture the enhanced, wave-induced transport which is otherwise not present in the simplified model anymore. Suitable models, localised in time and space, have to be developed for such transport coefficients to support equipment design.

The identification of a transport coefficient model in the transient, three-dimensional flat-film model represents a complex, strongly nonlinear inverse problem. Its direct solution is not attainable, since a suitable model structure is not known and good initial values for parameter estimation are typically lacking [4]. Therefore, we alternatively introduce incremental identification, a general framework, which has been successfully applied in diverse applications (e.g. [5, 6, 7]) before. The main idea is the decomposition of the original problem in a series of easier to handle subproblems. This way, not only more trustworthy parameter estimates can be
accomplished for a given model structure, but also the selection of a suitable model structure can be dealt with efficiently in a transparent way. This method requires no a-priori knowledge on the transport mechanisms which are typically unknown in real applications [8, 9], but results in a best-performing model if informative experimental data are available. Such informative data are obtained from an experiment with optimally designed experimental conditions. In this paper, a novel and efficient approach to the design of optimal falling film experiments is presented, which has not been attempted before for this and similar problems.

Figure 1: Schematic presentation of the simplification of the real falling film problem (left) to the flat-film model problem (right).

This paper is organized as follows. In Section 2, we present the simplified flat-film model with an effective transport coefficient. In Section 3, we outline the main concept and the steps of incremental identification to deduce an effective transport coefficient model. The procedure for designing an optimal falling film experiment is explained in Section 4. Finally, a numerical case study is presented in Section 5 to illustrate the methodology. Section 6 gives some conclusions.

2 PROBLEM STATEMENT

Let, \( \Omega \in \mathbb{R}^3 \) be a computational domain corresponding to the flat-film geometry (cf. Fig. 1). Let boundary parts \( \Gamma_D \cup \Gamma_N = \partial \Omega \) denote the Dirichlet (index \( D \)) and Neumann (index \( N \)) parts of the boundary and \([t_0, t_f] \) the time interval of interest. Consider the balance equation [9]

\[
\rho \left( \frac{\partial u}{\partial t} + \mathbf{w} \cdot \nabla u \right) - \nabla \cdot \left( (a_{\text{mol}} + f_s(u, x, t, 0)) \nabla u \right) = 0, \quad (x, t) \in \Omega \times [t_0, t_f],
\]

with initial and boundary conditions

\[
\begin{align*}
  u(x, t) &= u_0(x), \quad x \in \Omega, \\
  u(x, t) &= g_D(x, t) , \quad (x, t) \in \Gamma_D \times [t_0, t_f], \\
  \frac{\partial u}{\partial \mathbf{n}}(x, t) &= g_N(x, t) , \quad (x, t) \in \Gamma_N \times [t_0, t_f].
\end{align*}
\]

The scalar state variable \( u(x, t) \) represents specific enthalpy or mass density in case of energy or mass transport, respectively. The vector field \( \mathbf{w}(x, t) \in \mathbb{R}^3 \) is the mass-averaged convection velocity, which is assumed to be known throughout this paper. \( \rho \) is the constant fluid density. The vector \( \mathbf{n} \) denotes the outer normal on the boundary \( \Gamma \).

The effective diffusive transport in the flat-film flow geometry \( \Omega \) comprises molecular and dispersive transport, the latter of which is induced by backmixing due to waves [3, 10]. The resulting transport coefficient \( a = a(x, t) \) represents the sum of these two contributions,
\[ a(x,t) = a_{\text{mol}} + f_w(u(x,t), \theta), \quad (x,t) \in \Omega \times (t_0, t_f], \]  

and is typically a function of the state. The \textit{molecular transport} is expressed by the \textit{constant}, typically \textit{known} molecular transport coefficient \( a_{\text{mol}} \). The \textit{unknown}, \textit{wavy transport} coefficient captures all remaining transport phenomena and is expressed by a scalar model \( f_w(u(x,t), \theta) \) depending on the state variable \( u \), space coordinate \( x \), time \( t \) and model parameters \( \theta \in \mathbb{R}^p \).

Let, \( u_w(x_j,t_{i}) \) be the given, high resolution measurement data at a finite set of space locations \( x_j \in \Omega \) and time instances \( t_{i} \in [t_0, t_f] \). Since no specific structure is available for the \textit{wavy transport model} \( f_w(u(x,t), \theta) \) (cf. Eqs. (1), (2), (3)), a (finite) set \( I \) of candidate structures \( f_{w,i}(u(x,t), \theta), i \in I \), derived from different hypotheses is considered. The \textit{best-performing} transport model \( f_{w,i_0}(u(x,t), \theta), i_0 \in I \), has to be chosen based on a reasonable measure of model validity. The identification problem is not only nonlinear, but also of combinatorial nature, because all candidate models in the set \( I \) have to be evaluated. Furthermore, since the existence of a solution of eqs. (1), (2) can not be guaranteed [11], an \textit{admissible} structure of the transport coefficient model has to be inferred from the measurements \( u_w(x_j,t_{i}) \).

3 \hspace{2cm} \textbf{INCREMENTAL IDENTIFICATION OF TRANSPORT MODELS}

The \textit{incremental model identification} procedure (cf. Figure 2) builds on the steps of \textit{incremental modelling}, where the model structure is refined step-by-step in a structured model development procedure [12]. The solution of the nested subproblems results in the systematic and rigorous identification of the best-performing model structure and its parameters. We briefly explain incremental modelling and identification, but refer for details to [8, 9, 12].

As illustrated in Figure 2, the balance equations are formulated after fixing the balance envelope in the first step of incremental modelling. Then, constitutive relations, e.g. suitable flux laws and transport coefficient models, are gradually refined in the following modelling steps. This way a transparent submodel selection process is implemented.

Incremental identification directly reflects these modelling steps and decomposes the problem of transport coefficient model identification in \textit{three identification steps} using high resolution measurement data \( u_w(x_j,t_{i}) \). In the \textit{first identification step B}, the (artificial) source \( F_w \) describing the \textit{unknown}, wave-induced transport, is introduced in Eq. (1) (cf. Figure 2) to be reconstructed as a \textit{function of space} \( x \) and time \( t \) using the measurements \( u_w(x_j,t_{i}) \) (cf. Figure 2).

In the \textit{second identification step BF}, a transport law is chosen to model the source \( F_w \) such as, e.g., Fourier’s law in case of heat transport, or Fick’s law in case of mass transport. A \textit{wavy transport coefficient} \( a_w \) is introduced which again has to be reconstructed as a \textit{function of space} \( x \) and time \( t \) from the previously identified source data \( F_w'(x,t) \) (cf. Figure 2) interpreted as \textit{inferential} measurements. Since diffusive transport is time-invariant (i) the decoupling of space and time in the source, \( F_w'(x,t) = F_w'(x) \), \( \forall t \in [t_0, t_f] \), and in the wavy transport coefficient, \( a_w'(x,t) := a_w(x,t), \forall t \in [t_0, t_f] \), is introduced, (ii) the wavy transport coefficients are reconstructed as functions of \( x \) at each time instance \( t \), and (iii) the resulting functions \( a_w'^{i}(x) \) are assembled back to result in the transport coefficient function \( a_w'(x,t) = a_w'^{i}(x), \forall t \in [t_0, t_f] \) (cf. Figure 2). In the \textit{third identification step BFT}, this function is used as \textit{inferential} measurement data for the (manual) \textit{generation} of a set of candidate models \( f_{w,i}(u(x,t), \theta), i \in I \). The parameters of all these models are then estimated using \( a_w'(x,t) \) as \textit{inferential} measurement. In the final step, the best-
performing model \( f_{\theta_0}(u, x, t, \theta_0) \), \( i_0 \in I \), is selected using Akaike’s information criterion to obtain a model structure with the best fit and the smallest number of parameters [13].

Thus, while incremental modelling supports the transparent selection of suitable models in the intermediate steps, incremental identification efficiently decouples the identification problem in a sequence of affine-linear (step \( B \)), steady-state nonlinear (step \( BF \)) and algebraic (step \( BFT \)) subproblems. Since uncertainty is limited in each step, a more reliable identification of the best-performing model can systematically be achieved. Note, that the compilation of candidate model structures is supported by visual inspection of the wavy transport coefficient available from the first two steps. This is in contrast to the common simultaneous identification framework, where the transport coefficient model has to be directly identified from the fully specified model (1), which results from an aggregation of the assumptions on the flux and transport coefficient models. Hence, identification is simultaneously influenced by all assumptions made. The unavoidable uncertainty in the model structure increases the risk of poor estimates [4].

Incremental identification suffers from the disadvantage of error propagation, which results from the sequential solution of the inverse subproblems. However, this error can be efficiently corrected [9]. First, the transport coefficient \( a(x, t) \) (cf. Eq. (3)) is corrected by combining steps \( B \) and \( BF \) of incremental identification (cf. Figure 2) into one. The corrected transport coefficient is then used in the third step \( BFT \) to correct the selection of the transport coefficient model structure.

4 OPTIMAL DESIGN OF EXPERIMENTS

This section briefly describes the strategy for designing optimal experiments for an accurate identification of a transport coefficient model. To this end, an optimal experiment for parameter precision has to be determined which results in measurement data with sufficient information content, measured by the determinant of the Fisher information matrix [14].

In particular, an optimal experiment is designed for the reconstruction of the transport coefficient \( a(x, t) \) as a function of space \( x \) and time \( t \) in Eq. (3). A maximization problem is formulated with selected experimental conditions as the degrees of freedom, the determinant of the Fisher matrix as the objective function, and the transport model Eqw. (1)-(3) as the constraint. A reasonable reference value is chosen for the unknown transport coefficient (for example, a constant, cf. Section 5) to fully specify the transport model. The Fisher information matrix requires the computation of the sensitivities of the measurements (here the full state \( u(x, t) \)) with respect to the unknown model parameters. Since a model of the transport coefficient is not available, the function \( a(x, t) \) is represented by its discretization. A fixed coarse spatial mesh continuously propagated in time is chosen which can capture the spatial localization of the
unknown transport coefficient with sufficient accuracy. The sensitivity of the system state with respect to the transport coefficient is calculated as the directional derivatives of $u(x,t)$ with respect to $a(x,t)$ in the direction of the unit vectors in each mesh point. These sensitivities follow from a solution of the sensitivity problem associated with Eqs. (1)-(3). The choice of a coarse mesh limits the computational cost for the solution of the experiment design problem, but still results in an informative experiment.

The optimally designed experiment is carried out. The measured data are then used for the identification of a transport coefficient model applying the incremental identification method [8] including the model correction step [9] as described in the previous section.

5 NUMERICAL CASE STUDY

The numerical case study assumes an exact realization of the transport coefficient in Eq. (3) as shown in Figure 3. The Dirichlet boundary $\Gamma_D$ functions $g_D^\in$ at the inlet $\Gamma_a$ and $g_D^{wall}$ at the wall $\Gamma_{wall}$ (cf. Figure 1 and (2)), and the geometric parameters of the falling film geometry, i.e., the thickness $\delta_o$ and length $L_x$ of the falling film (cf. Figure 1) are chosen as the experimental conditions to be designed optimally. The determinant of the Fisher information matrix is computed as described in Section 4 for varying experimental conditions and the nominal value for the unknown diffusion transport coefficient $a_0$ corresponding to the constant initial value depicted in Figure 3. The optimal experiment results in the boundary functions $g_D^\in(x,t) = \left[-10 \frac{y}{\delta_o} + 20\right][^\circ C]$ and $g_D^{wall}(x,t) = \left[50 \left(1 - \cos \left(\frac{\pi x}{L_x}\right)\right) + 20\right][^\circ C]$, the film thickness $\delta_o = 0.015$ [mm] and the film flow length $L_x = 0.1$ [mm]. Using this experimental setup, we generate simulated measurement data by simulating the designed experiment using the (exact) diffusion coefficient shown in Figure 3. Additionally, these data are perturbed artificially.

Figure 3: Estimated best transport coefficient model for $y = 0.0075$ [mm] and $z = 0.01$ [mm], $y = 0.005$ [mm] and $z = 0.01$ [mm]; non-optimally designed experiment.

Figure 4: Estimated transport coefficient model for model for $y = 0.0075$ [mm] and $z = 0.01$ [mm], $y = 0.005$ [mm] and $z = 0.01$ [mm]; non-optimally designed experiment.

Figure 3 shows the results of the identification of the transport coefficient model from the optimally designed experiment. In addition to the constant initial estimate and the exact transport coefficient, the Figure shows the model-free estimate of the transport coefficient resulting from the correction step (cf. Section 3) and the parametric transport coefficient model selected from a set of seven candidate model structures (see [9] for details). The selected model structure and its associated estimated parameters minimize Akaike’s information criterion for all the candidates in the set. To demonstrate the potential and the necessity of an optimally designed experiment, Figure 4 presents the identification results obtained from a non-optimal experiment. The lack of estimation quality can be readily observed. Moreover, the estimate is unstable as a consequence of the measurement errors.
6 CONCLUSIONS

A rigorous method for the incremental identification of a transport coefficient model in a flat-film model of a wavy falling film comprising a transient convection-diffusion equation in three space dimensions is presented. The simultaneous identification problem is split into three hierarchically structured subproblems which are solved sequentially. After a model-free estimation of the transport coefficient, the most suitable parametric model structure is selected from a set of candidates using Akaike’s information criterion. The novel contribution in this paper is the optimal design of experiments for parameter precision. The maximization of the information content of the measurements results in a most informative experiment, which is essential for the identification of an accurate transport coefficient model. An illustrative numerical case study reveals the potential and the necessity of optimal design of experiment for a reliable identification of distributed parameter systems, and in particular, for the flat-film model of a wavy falling film.

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