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Optimal experimental design for identification of transport coefficient models in convection–diffusion equations

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ABSTRACT

Methods for the careful design of optimal experiments for the identification of the structure and parameters of transport models often strongly depend on a-priori knowledge about the unknown model. However, this kind of knowledge is usually poor for complex systems. We propose a novel procedure that is less sensitive with respect to poor a-priori knowledge; it relies on an optimization problem to maximize the information content of the measurement data for the purpose of model identification. Specifically, based on existing model-based methods, optimal design of experiments is addressed in the context of three-dimensional, time-dependent transport problems by introducing experiment design variables and the transport coefficient as degrees of freedom of the optimization. The problem is solved by means of an iterative strategy that – by sequentially designing a series of experiments – strives to adjust the settings of the experimental conditions by exploiting the results from previous experiments.

The key methodical ingredient of the novel procedure is the use of incremental model identification introduced previously. The suggested procedure is illustrated by means of an extensive numerical case study for a convection–diffusion equation originating from the modeling and simulation of energy transport in laminar wavy film flow.

1. Introduction

This work studies optimal experimental design (OED) for the identification of the structure and the parameters of transport coefficient models in laminar wavy film flows. Falling film flows occur in many multi-phase unit operations such as falling film reactors, falling film evaporators, absorption columns, two-phase flow reactors or falling film micro-separators and reactors (cf., e.g., Chasanis et al., 2010).

Instability and complex dynamics of developing surface waves that are characteristic for falling film flows (cf. e.g., Meza and Balakotaiah, 2008) make the direct numerical simulation of the dynamical flow model in three space dimensions extremely demanding, both, from a numerical and a computational point of view. Therefore, simplified flow models are often preferred in practice. Such models reduce the original two-phase flow problem with dynamical, free boundary to a *single*-phase film flow problem with a *known* and stationary or slowly varying boundary (cf. e.g. Wilke, 1962). *Effective* transport coefficients are introduced to compensate the errors unavoidably resulting from such simplification and to capture the enhanced, wave-induced transport effects localized in space and in time. To support equipment design, these transport coefficients are parametrized and calibrated using transport models with a low number of parameters. Note, that no specific model structure of such a transport model is available. It rather has to be inferred from measurement data.

Let us consider the following transport model to approximate the behavior of laminar wavy film flows. Let $\Omega \subset \mathbb{R}^3$ be a rectangular computational domain corresponding to a *reduced* flow geometry, i.e., $\Omega := (0, L_x) \times (0, \delta_0) \times (0, L_z)$ with the dimensions L_x, δ_0 and L_z in x, y and z space coordinates, respectively. Let the boundary $\Gamma_D \cup \Gamma_N = \partial\Omega := \Gamma$ be composed of the Dirichlet (index D) and Neumann (index N) parts of the boundary, respectively, and let $[t_0, t_f]$ be the time interval of interest. Consider the balance equation

$$\rho(\frac{\partial u}{\partial t} + \mathbf{w} \cdot \nabla u) - \nabla \cdot ((a_{\mathrm{mol}} + a_w(\mathbf{x}, t))\nabla u) = 0, \ (\mathbf{x}, t) \in \Omega \times (t_0, t_f], \tag{1a}$$

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with initial and boundary conditions

$$\begin{aligned} u(\mathbf{x}, t_0) &= u_0(\mathbf{x}), \quad \mathbf{x} \in \Omega, \\ u(\mathbf{x}, t) &= g_D(\mathbf{x}, t), \quad (\mathbf{x}, t) \in \Gamma_D \times [t_0, t_f], \\ \frac{\partial u}{\partial \mathbf{n}}(\mathbf{x}, t) &= g_N(\mathbf{x}, t), \quad (\mathbf{x}, t) \in \Gamma_N \times [t_0, t_f]. \end{aligned} \tag{1b}$$

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

The effective transport distinguishes between different transport mechanisms. Specifically, the molecular transport is expressed by the constant and known molecular transport coefficient a_{mol} corresponding to the thermal properties of the fluid. Whereas, *unknown* transport induced by waves (Brauer, 1956; Wilke, 1962) captures all remaining transport enhancing effects and is expressed by the *wavy* transport coefficient $a_w(\mathbf{x}, t)$,– a function of space and time coordinates $\mathbf{x}$ and t. We assume the effective transport to be constant near the boundary Γ, such that the boundary condition given at Γ_N in Eq. (1b) is well-defined.

The wavy transport coefficient function is parametrized using a transport model function $f_w(u, \mathbf{x}, t, \boldsymbol{\theta})$ of the state variable u, space and time coordinates $\mathbf{x}$ and t, and model parameters $\boldsymbol{\theta} \in \mathbb{R}^p$, $p \in \mathbb{N}$.[4] A set of reasonable candidate model structures (derived from different physical or theoretical insights) with typically less than, say, ten parameters is assumed to be available. After estimation of each candidate model from this set, the best-suited one – $f_w^\star(u, \mathbf{x}, t, \boldsymbol{\theta})$ – has to be chosen, relying on some statistical measure of goodness of fit.

The development and identification of $f_w^\star(u, \mathbf{x}, t, \boldsymbol{\theta})$ from transient, distributed measurements $u_m(\mathbf{x}_j, t_k)$ describing energy or mass transport at a finite set of sampling points $(\mathbf{x}_j, t_k) \in \Omega \times [t_0, t_f]$ has been studied in detail by the authors before (Karalashvili et al., 2008, 2011). That work relied on the *incremental model identification* method, which decomposes the nonlinear model identification problem in a series of subproblems. The main strengths of this method are (i) it does not require any a priori knowledge on the unknown transport model structure, (ii) due to the decomposition, it supports a systematic transport model identification process, and finally (iii) it allows for a rigorous decision making on the best-suited model structure from the given candidate set. Yet, our extensive numerical studies revealed that the experiment conditions defined by, e.g. experiment duration, initial and/or boundary conditions, geometrical dimensions of the computational domain etc., dramatically affect the overall identification process and strongly influence the quality of the results. These findings motivated us to explore the design of optimal falling film experiments (Karalashvili, 2012).

Obviously, the quality of identified transport model is limited by: the nonlinearity of model, inevitable errors in the experimental data and the correlation in model parameters (cf. e.g. Beck and Woodbury, 1998; Emery and Nenarokomov, 1998; Walter and Pronzato, 1997). Hence, any identification method is challenged in finding a good solution, since multiple local solutions of the estimation problem may exist. Therefore, the OED problem may not be approached without addressing the question: are transport coefficients identifiable from the available measurement data? This question is a subject of identifiability study.

Model-based methods for OED are able to effectively address the problems discussed above (Walter and Pronzato, 1997). Specifically, experiments should be designed such that the subsequent identification of transport coefficient models results in model parameters with maximum precision. In other words, an optimal experiment should provide the most informative measurement data, that in some sense, guarantees model and parameter identifiability and results in parameter estimates of minimal uncertainty. This requires an assessment of the measurement data quality.

To assess the information content of the measurement data, the Fisher information matrix (FIM) is commonly used as a quantitative measure (Fisher, 1992). FIM is related to the expected accuracy of the estimates. It quantifies the sensitivity of the measured system states with respect to the model parameters and hence holds information on the degree of parameter correlation. Consequently, settings resulting in a loss of parameter identifiability can be avoided (cf., e.g., Emery and Nenarokomov, 1998; Leontaritis and Billings, 1987; Point et al., 1996; Walter and Pronzato, 1997).

The use of FIM for OED of distributed parameter systems is not a new concept (cf., e.g., Alifanov et al., 1995; Anderson et al., 2005; Emery and Nenarokomov, 1998; Emery, 1999; Fadale et al., 1995; Point et al., 1996; Ranjbar et al., 2009; Sun, 2005; Uciński, 2005; Wouwer et al., 2000 and references therein). However, application of this theory to problems in two or three space dimension is relatively rare (cf., e.g., Anderson et al., 2005; Emery and Nenarokomov, 1998; Uciński, 2005). Moreover, only very few works address transient problems (e.g., Uciński, 2005). Furthermore, these studies rely on a fixed, known model structure and assume good a-priori estimates for the model parameters.

In this work, we propose a sequential procedure, which allows for model-based design of optimal falling film experiments for precise identification of the structure and the parameters of the transport coefficient $a_w(\mathbf{x}, t)$ in problem (1). In contrast to the existing literature, we do not rely on the known model structure for the transport coefficient.

The paper is structured as follows. In Section 2, we explain the incremental model identification method very briefly. The decomposition steps of this method build the key methodical ingredient of the novel OED procedure. In Section 3, we mathematically state the OED problem and address all necessary constructs and concepts. Section 4 presents the sequential design procedure in details. Section 5, illustrates it on an extensive numerical case study and finally, in Section 6, significant conclusions are presented and future steps are outlined.

2. Incremental model identification

The incremental model identification method applied to the identification of transport coefficient models in systems of convection–diffusion type studied in this work (cf. Eq. (1)) is given in Fig. 1.

The key idea of the incremental model identification approach is the gradual refinement of the model structure during identification by reflecting the incremental steps which are common in model development. According to the model development procedure proposed by Marquardt (1995), the model structure is refined step-by-step, starting from the (mass or energy) balance equations (model *B*). Source models (model *BF*) and transport coefficient functions (model *BFT*) are introduced subsequently. This way, the choice of the transport model (e.g., Fick's or Fourier's law) and the choice and parameterization of the transport coefficient functions

[3] The flow velocity can be measured.

[4] Note that, in general, the transport model f_w depends also on the flow velocity $\mathbf{w}$, which, as reported, is assumed to be known throughout the paper. For more general presentation, we use the notation $f_w(u, \mathbf{x}, t, \boldsymbol{\theta})$ to underline the dependence of this model on the state u, even though we do not consider the dependency of the wavy transport coefficient function $a_w(\mathbf{x}, t)$ on the state u to milden the nonlinearity in the model (1).