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Incremental identification of transport phenomena in wavy films

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Abstract

The complexity of wavy film flows results in a high computational cost for a direct numerical simulation. Simplified models are therefore attractive alternatives for engineering design calculations. An incremental approach for the identification of transport models in wavy film flows is presented here. The proposed strategy decomposes the identification problem into a series of sequential, computationally easier to handle inverse problems. The proposed methodology is illustrated for the identification of an energy transport model in a wavy film. The first step of such an incremental identification approach is carried out on a case study.

Keywords

Modelling, identification, high resolution measurement data, parameter estimation, inverse problem, regularization

1. Introduction

The modelling of transport phenomena in wavy film flows is an active area of research due to the technical relevance and the numerous applications of such flows in process and energy engineering (cf. [1] and the references therein). Hence, the development of computationally manageable models, yet accurately describing the underlying transport processes is very important for the design of technical systems.

The structure of a the model is usually inferred by combining experimental data with results of theoretical analyses. Moreover, several competing model structures may exist. The most commonly used simultaneous identification strategy, aggregates the model candidates for the individual phenomena with the balance equations to result in the complete model of the wavy film flow. Measurement data are used to estimate the unknown parameters and to discriminate between competing submodels. This approach seems to be too complex and little promising, since on the one hand, a large number of estimation problems with many unknown parameters have to be solved and on the other hand, the insertion of an unsuitable submodel into the balance equations may result in a biased model [2]. In contrast, the incremental identification strategy [3], where the model structure is gradually refined, is a robust and efficient alternative (cf. [3] and the references therein). In this paper, the incremental approach of model identification is applied to transport phenomena in wavy films.

In the next sections, the incremental procedure for the identification of energy transport in a wavy film is described and formulated as a set of sequential inverse problems. Then, the numerical solution strategy for the first incremental step is outlined. A case study is performed to illustrate and benchmark the proposed method in simulation. Finally, conclusions and remarks concerning future work are given.

2. Incremental Model Development

The major reason for the huge computational costs of direct transient numerical simulations of wavy film flows lies in the multiphase character of such flows. In order to reduce the problem complexity, the 3-dimensional (3D) time-varying domain corresponding to the liquid phase is mapped to a 3D time-invariant waveless domain $\Omega_{FF} \subset R^3$. While doing so, a space- and time-dependent *effective transport coefficient* is introduced [4] to capture all wave-induced transport effects in the reduced flat film (FF) geometry.

Model development is commonly performed in incremental steps starting with the formulation of the balance equations [5]. Consider for example, the energy transport model for a pure component incompressible fluid. In a first step, the energy balance (model B) without sources can then be written as

$$\textit{model B:} \quad \rho c\left(\frac{\partial T}{\partial t} + \mathbf{u}\cdot\nabla T\right) = -\nabla\cdot q\,, \qquad (\mathbf{x},t)\in\Omega_{FF}\times[t_0,t_f]\,. \tag{1}$$

$T(\mathbf{x},t)$ and $q(\mathbf{x},t)$ are the temperature and heat flux, respectively; t_0 and t_f denote the initial and final times; ρ and c represent constant density and thermal capacity of the fluid, respectively. The velocity field $\mathbf{u}(\mathbf{x},t)$ is assumed to be known. In the next step, a constitutive model for the heat flux $q(\mathbf{x},t)$ such as Fourier's law, e.g.

$$\textit{model F:} \quad q = -\rho c a_{\text{eff}} \nabla T \tag{2}$$

is chosen. Here, $a_{\text{eff}}(\mathbf{x},t)$ stands for the effective thermal diffusivity. In the final step of the incremental modelling procedure (model BFE), the effective thermal diffusivity has to be correlated with states (e.g. temperature, velocity etc.) and model parameters to close the model.

3. Incremental Model Identification

The key idea of incremental model identification is to use the same sequence of steps as in incremental model development. Assume, we have a measurement system providing temperature measurement data at high resolution in time t and space $\mathbf{x}$. The incremental identification of the energy transport model can be carried out as shown in Fig.1.

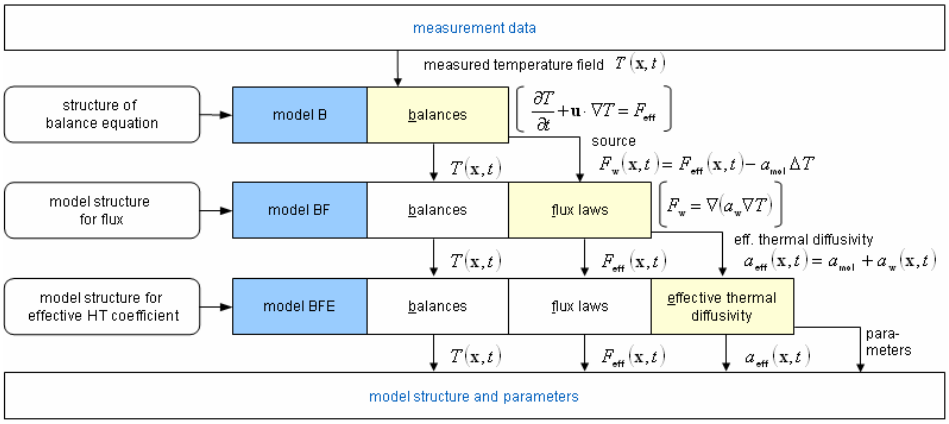

Fig.1: Incremental identification of heat transport in wavy films

First, the effective source term $F_{\text{eff}}(\mathbf{x},t) \equiv \nabla q$ in model B, the energy balance (1), is estimated as a function of space $\mathbf{x}$ and time t, under the assumption that the remaining initial and boundary conditions are known. This is a typical inverse problem, which is ill-posed and should be appropriately regularized. Since (1) represents a convection equation, the choice of boundary conditions is restricted. Furthermore, such convection equations are in general harder to treat numerically than problems in which diffusion phenomena are present, too. Therefore, the following decomposition of F_{eff} is proposed. From a physical point of view, it is reasonable to split the effective thermal diffusivity into two contributions according to

$$a_{\mathbf{eff}}(\mathbf{x},t) = a_{\mathbf{mol}} + a_{\mathrm{w}}(\mathbf{x},t) \tag{3}$$

where $a_{\mathbf{mol}} = \lambda/\rho c = const.$ is the constant *molecular thermal diffusivity* corresponding to the material properties of the fluid and $a_{\mathrm{w}}(\mathbf{x},t)$ expresses the wave-induced effects in the model FF considered. This ansatz induces a splitting of the effective source term to result in $F_{\mathbf{eff}}(\mathbf{x},t) = a_{\mathbf{mol}}\Delta T + F_{\mathrm{w}}(\mathbf{x},t)$. As a consequence, the wave induced part of the effective source term $F_{\mathrm{w}}(\mathbf{x},t)$ is estimated instead of $F_{\mathbf{eff}}(\mathbf{x},t)$ (cf. Fig 1.). The *direct problem* then consists of a transient *convection-diffusion* equation for the temperature T

$$\frac{\partial T}{\partial t} + \mathbf{u}\cdot\nabla T - a_{\mathbf{mol}}\Delta T = F_{\mathrm{w}}, \qquad (\mathbf{x},t)\in\Omega_{FF}\times(t_0,t_f], \tag{4}$$

with suitable initial and boundary conditions. This problem is numerically easier to treat than (1) as it allows the use of Neumann boundary conditions at the interface between the film and the heater.

The estimation of the function $F_{\mathrm{w}}(\mathbf{x},t), (\mathbf{x},t)\in\Omega_{FF}\times[t_0,t_f]$ on the basis of available measurement data $T_m(\mathbf{x},t)$ in $\Omega_{FF}\times[t_0,t_f]$ leads to an *inverse problem.* A solution strategy for this problem is considered in Section 4. Using the estimated wavy-part $F_{\mathrm{w}}(\mathbf{x},t)$ of the effective source term, in model BF, cf. Fig. 1, the effective thermal diffusivity can be reconstructed using (3) by solving, for each time step, an appropriate steady-state inverse problem for $a_{\mathrm{w}}(\mathbf{x},t)$.

4. Estimation of source term $F_{\mathrm{w}}(\mathbf{x},t)$

The inverse problem for reconstruction of $F_{\mathrm{w}}(\mathbf{x},t)$ is stated as an optimization problem: *determine the unknown quantity $F_{\mathrm{w}}(\mathbf{x},t)$ such, that the residual*

$$J(F_{\mathrm{w}}) = \frac{1}{2}\int_{t_0}^{t_f}\int_{\Omega_{FF}}\left[T(\mathbf{x},t;F_{\mathrm{w}}) - T_m(\mathbf{x},t)\right]^2 d\mathbf{x}dt \to \min \tag{5}$$

where $T(\mathbf{x},t;F_{\mathrm{w}})$ satisfies the direct problem (4).

The solution strategy is based on [6], where a conjugate gradient (CG) method is employed to solve a similar inverse problem. An initial approximation of the unknown quantity $F_{\mathrm{w}}^{\mathbf{0}}(\mathbf{x},t)$ is chosen, which is updated during an iterative process, while moving along a descent direction with an optimal step length. As the direct problem (4) is affine-linear, in each step of the iteration only *two* direct transient convection-diffusion problems – the *adjoint* and the *sensitivity* problems have to be solved in order to analytically determine the descent direction and step length [6]. The direct adjoint and sensitivity problems are solved using the software package DROPS [6], which is based on multilevel nested grids and finite-element discretization methods.

Regularization is implicitly introduced via the discretization and is explicitly implemented by means of a suitable stopping criterion for the iterative process. The number of CG-iterations serves as a regularization parameter. The value for this parameter is determined either by the discrepancy principle or the L-curve method [7].

5. Illustrative case study

The domain $\Omega_{FF} = \left[\, 0.18 \times 3 \cdot 10^{-3} \times 3 \cdot 10^{-3} \,\right] m^3$ is considered. Here, x is the flow direction of the falling film and y is the direction along the film thickness. The material properties of the fluid are lumped in the parameter $a_{\mathbf{mol}} = 8.4 \cdot 10^{-8}\ m^2/\mathrm{sec}$. The time interval $[0{,}2\,\mathrm{sec}]$ is discretized with the step size $\Delta t = 0.01\,\mathrm{sec}$. The known constant initial and boundary conditions are $T(\mathbf{x}, t_0) = 20^\circ C,\ \mathbf{x} \in \Omega_{FF}$; $T_{in}(\mathbf{x}, t) = 20^\circ C, (\mathbf{x}, t) \in \Gamma_{in} \times [t_0, t_f]$; $q_h(\mathbf{x}, t) = 4960\, kW/m^2$, $(\mathbf{x}, t) \in \Gamma_{heat} \times [t_0, t_f]$. The optimization procedure is initialized by $F_{\mathbf{w}}^0 = 0,\ (\mathbf{x}, t) \in \Omega_{FF} \times [t_0, t_f]$.

The effective wave-induced source term to be estimated in the first step of the incremental model identification approach is chosen as

$$F_{\mathbf{w}}^{ex}(x, y, z; t) = x\left[\sin\left(6\pi\left(\frac{x}{180} + t\right)\right) + \frac{y}{0.3} \cdot t + \frac{z}{0.3}\right], (x, y, z) \in \Omega_{FF}, t \in [t_0, t_f].$$

Artificially perturbed temperature measurements according to

$$T_m = T_m^{ex} + \sigma\varpi$$

are assumed to be available, where $T_m^{ex}(\mathbf{x}, t)$ is the temperature obtained from the solution of the direct problem (4) with $F_{\mathbf{w}}^{ex}(\mathbf{x}, t)$ given above as a right hand side. σ represents the standard deviation of the measurement error. Values of ϖ are generated from the zero mean normal distribution with variance one.

The discrepancy principle is used as stopping rule, i.e. the CG iteration is stopped if the condition $J(F_{\mathbf{w}}^{n_{opt}}) < \kappa(t_f - t_0)V\sigma$ is fulfilled, with V being the volume of Ω_{FF} and $\kappa > 1$ [7]. For $\kappa = 1.02$, the solution is found after $n_{opt} = 47$ iterations. The exact and estimated source terms for time $t = 0.75\,\mathrm{sec}$ are given in Fig. Similar results have been obtained using the L-curve.

The recovered source term is in good agreement with the exact one, except for the part near the outflow boundary $x = 180\, mm$. The large differences there are caused by the lack of information due to the convection. Large errors occur also close to the final time, due to the fact that the gradient of the objective functional is zero and thus causes no improvement of the initial approximation.

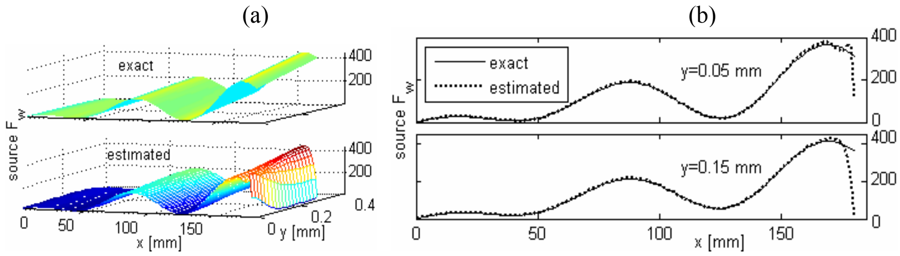

Fig.2: Exact and estimated source F_w for constant $z = 0.15\ mm$ with perturbed measurements $\sigma = 0.25$ at $n_{opt} = 47$ (a) over x and y directions (b) over x direction for different y.

6. Conclusions and future work

The incremental approach for the estimation of an effective transport coefficient in a flat film decouples the computationally expensive estimation problem into sub problems, which are much easier to solve. The overall computational cost is considerably reduced, as different submodel candidates have to be investigated repeatedly only at the second and third steps. The first step of the incremental approach has been studied and validated. In future work, the second and third steps will be performed (cf. Fig. 1). The whole incremental procedure will be studied and examined both for simulated and real measurement data. Also, error propagation due to the sequential solution of a series of inverse problems will be analyzed.

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