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An improved scaling procedure for analysis and simplification of process models

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ABSTRACT

Systematic scaling analysis of model equations can be valuable as a tool for developing computationally tractable simulations of physical systems. The scaling analysis methods in literature pose difficulties in the calculation of scale and reference values, when nonlinear terms are involved in the model equations. Further, existing methods involve trial and error procedures in the scaling process. In this paper, a systematic approach for handling nonlinear terms is suggested, which results in appropriate scale and reference values that render the dimensionless variable variations to be of order one. Further, trial and error procedures are avoided through a new approach wherein a set of nonlinear algebraic equations are solved to identify the scale and reference values. The proposed scaling approach is common to any given model equations with fixed parameters. However, it is to be noted that the proposed procedure may not handle situations when model equations exhibit steady state multiplicity and have dynamic multi-mode regimes. The proposed scaling procedure is illustrated through various examples of different complexities. A 1D model of WGS reactor as a case study shows the effectiveness of the obtained scale and reference values in obtaining simplified model which represents the steady state and dynamic variations of the variables.

1. Introduction

Scaling analysis is a systematic approach that can be used to identify phenomena occurring at various scales. This information can be used to simplify a given set of equations by neglecting phenomena, which occur at scales that are different from the scale of interest. In this approach, a given set of equations is made dimensionless, resulting in several dimensionless groups of varying magnitudes. These dimensionless groups represent the relative effects of phenomena or mechanisms and therefore help identify dominant phenomena/mechanisms in the scale of interest. A number of authors have used scaling analysis for model simplification and identification. For example, Dahl et al. (2004) have used scaling analysis to get insights into the behavior of fluid aerosol reactor without performing actual simulations. Kopaygorodsky et al. (2004) have used scaling analysis to identify key differences between the modeling assumptions for conventional pressure swing adsorption and ultra-rapid pressure swing adsorption. Kaisare et al. (2005) have used scaling analysis to identify phenomena occurring at varying scales in a reverse flow reactor. Balaji et al. (2008) have used scaling analysis for reverse flow reactor and have shown ways of simplifying the model equations. Rao et al. (2010) have used scaling analysis

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for pulsed pressure swing adsorber to identify useful correlations in terms of dimensionless numbers. Rezvanpour et al. (2012) have studied electro-hydrodynamic atomization process using scaling analysis to simply the model and to find a correlation relating efficiency with a single dimensionless number involving the parameters of the process. Baldea and Daoutidis (2007) have used scaling analysis for auto-thermal reactors to identify a non-stiff model by separating fast and slow time scales. Krantz (2007) have described the method of scaling analysis in a book for various transport and reaction process.

There are two important gaps in all these works that use scaling analysis. In the scaling methodology described by Krantz (2007), all dependent and independent variables in the equations are made dimensionless by choosing appropriate scale(s) and reference factor(s). This results in a minimum parametric representation of the model equations. Thus the solution of these equations can be expressed in terms of dimensionless groups. The form of these dimensionless groups and the methods used for obtaining scales usually involve trial and error methods. In Krantz et al. (2012), it is mentioned that one has to know the controlling mechanism while forming a unique dimensionless equation which varies in the order of 1. Identifying this controlling mechanism is not obvious and in most cases this usually involves a trial and error process. Further, in all these works on scaling analysis, the scaling of nonlinear terms in the equations is addressed in an empirical manner. The scale for nonlinear terms are usually taken to be some characteristic maximum (Balaji et al., 2008; Krantz, 2007), but obtaining this maximum is not obvious without simulating the corresponding equations. We address these gaps in the literature by: (i) proposing an approach that avoids the trial-and-error method for deriving scales, and (ii) we focus on nonlinear terms and suggest a systematic way to obtain appropriate scales for these terms. The proposed method for scaling analysis is general and straight-forward to apply to any given set of equations. The proposed method is described in several steps and explained though examples of varying complexity. We apply the techniques developed in this paper and calculate scale and reference values for a 1D model of water gas shift (WGS) reactor system, which involves complex nonlinear terms and differential algebraic equations. The obtained scale and reference values are shown to be appropriate in making the corresponding dimensionless variables to vary in the order of 1. Analysis of obtained scale and reference values through relevant dimensionless groups results in a simplified model. The performance of the simplified model based on these scales is evaluated by comparing the simulation results with a detailed model and bench-marking the respective computational performances.

2. Model simplification using current method of scaling analysis

Systematic scaling analysis of model equations can identify phenomena with varying importance thereby providing a rational approach for model simplification through elimination of terms and elimination of equations with minimal impact on the simulation results. Scaling analysis involves identifying appropriate scale and reference values to make the entire dependent and independent variables in a model to be dimensionless and vary in the order of 1, i.e. these dimensionless variables vary from zero to near one. This type of representation for a model is termed as minimum parametric representation. In this representation, it is easy to identify terms (which corresponds to some physical phenomenon) of least importance and one can discard them to obtain a simplified model.

In this section we first provide a general description of the scaling analysis and point out the deficiencies in the existing procedures at appropriate places. The method of scaling analysis followed in the literature is described below through several steps using a simple example.

Step 1: Consider the following system of equations

$$\frac{dy_1}{dx} = f_{11}(y_1, y_2, x) + f_{12}(y_1, y_2, x) \tag{1}$$

$$\frac{dy_2}{dx} = f_{21}(y_1, y_2, x) + f_{22}(y_1, y_2, x) \tag{2}$$

The initial conditions for the above equations are given by

$$y_1(x = 0) = y_{10}; \quad y_2(x = 0) = y_{20} \tag{3}$$

Step 2: Define dimensionless quantities (involving scale and reference values) for dependent and independent variables and introduce them into the equations

$$y_1^* \equiv \frac{(y_1 - y_{1,r})}{y_{1,s}}; \quad y_2^* \equiv \frac{(y_2 - y_{2,r})}{y_{2,s}}; \quad x^* \equiv \frac{x}{x_s} \tag{4}$$

In the above definition, variables with subscript 's' and 'r' represent scale and reference values respectively and variables with superscript '*' represent dimensionless quantities. Reference and scale values are introduced so that resulting dimensionless variable starts from zero and vary in order of 1 respectively. This means reference value is required only for variables which are not starting from zero. Hence in the above example, reference value is not introduced in the definition for dimensionless independent variable. However there are situations (for example, for fluid flow problem involving annulus pipe) where independent variables does not start from zero and in those situations one need to have reference values. Introducing these definitions in Eqs. (1)–(3)

$$\frac{y_{1,s}}{x_s}\frac{dy_1^*}{dx^*} = f_{11}(y_1^* y_{1,s} + y_{1,r}, y_2^* y_{2,s} + y_{2,r}, x^* x_s) + f_{12}(y_1^* y_{1,s} + y_{1,r}, y_2^* y_{2,s} + y_{2,r}, x^* x_s) \tag{5}$$

$$\frac{y_{2,s}}{x_s}\frac{dy_2^*}{dx^*} = f_{21}(y_1^* y_{1,s} + y_{1,r}, y_2^* y_{2,s} + y_{2,r}, x^* x_s) + f_{22}(y_1^* y_{1,s} + y_{1,r}, y_2^* y_{2,s} + y_{2,r}, x^* x_s) \tag{6}$$

$$y_1^*(x^* x_s = 0) = \frac{(y_{10} - y_{1,r})}{y_{1,s}}; \quad y_2^*(x^* x_s = 0) = \frac{(y_{20} - y_{2,r})}{y_{2,s}} \tag{7}$$

In the above equations, (f_{11}, f_{12}, f_{21}, f_{22}) can represent linear or nonlinear terms involving dependent and independent variables. For these terms, once appropriate dimensionless variable definitions are introduced, one should be able to separate them into terms involving only scale and reference values and terms involving only dimensionless variables. For example, after scaling the term f_{11}, this needs to be written as a product of two terms $f_{11,s} = f_{11}(y_{1,s}, y_{1,r}, y_{2,s}, y_{2,r}, x_s, x_r)$ and $f_{11}^* = f_{11}(y_1^*, y_2^*, x^*)$. This separation becomes difficult for most of the nonlinear terms and there is hardly any work in the