MODELING AND MODEL CALIBRATION OF COMPLEX DYNAMICAL SYSTEMS APPLIED TO THE PRIMARY CIRCUIT OF A NUCLEAR POWER PLANT

Theses of Ph.D. dissertation

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1 Motivation and goal

A model is an imitation of the reality and a mathematical model is a particular form of the representation [1]. In the process of model building we translate our real world problem into an equivalent mathematical problem which we solve and then attempt to interpret. We do this to gain insight into the original real world situation or to use the model for control, optimization, safety etc. studies.

The appropriate level of details of modeling is determined by the modeling goal. Because models act as bridges between levels of understanding, they must be detailed enough to make contact with the lower level yet simple enough to provide clear results at the higher level. It means that a good model satisfies the modeling goal and it is as simple as possible to make the understanding easier. Such a model is called *minimal model*.

The goal of this thesis is to construct minimal models, in a generalized sense, of special complex systems based on first engineering principles in order to apply these models for system analysis, model calibration, controller design and fault analysis. The approach of model building applied in this thesis is to use our physical knowledge about the system to construct its model. A special model construction procedure is presented tat results in a model composing from minimal elements on the primary circuit of a nuclear power plant.

The primary circuit of a nuclear power plant transfers the heat generated in the reactor to the secondary circuit and cools the reactor continuously [2]. The modernization of nuclear power plants requires a complete redesign of some of its parts, such as controllers of the primary circuit. To design good controllers we need a quite accurate, dynamic and yet simple model of the primary circuit. Therefore, the aim here has been to *develop a minimal, in a generalized sense, primary circuit model for controller design purposes. Parts of the model must have physical meaning and the model must represent all of the main dynamics of the real system*.

A complete model is required for any application, i.e. not just the model equations but the values of model parameters must be known. Therefore, the model calibration procedure also has to be completed during modeling that yields the estimated model parameters using measured data from the real system. To build complete primary circuit models, an important goal has been to *realize the model calibration procedure for the nonlinear model*.

In case of highly safety-critical and complex systems, such as a nuclear power plant, the verification and validation of the safety procedures is of great importance because it can provide the correct responses of the system to the possible faults. A nuclear power plant is called a safe system, if it can respond correctly to the faults in a predefined time limit. Because of the large number of variables and the complexity of the plant and its dynamical behavior, however, one needs to apply formal methods for this task. Therefore, the goal here has been to *develop a primary circuit model for fault analysis and verification of the recommended safety procedure.*

2 Methods and Tools

2.1 The seven-step modeling procedure

A recommended, iterative model development procedure [1] was used here that consisted of seven steps:

1. *Problem definition*. This defines the system, the modeling goal and the validation criteria. The definition of system means the definition of system boundaries and the way of interactions between the system and its environment together with the description of the internal structure of the system itself. Any model is developed for a specific use or uses that is determined by the modeling goal. Validation criteria determine when the modeling development cycle should terminate.

2. *Identify controlling factors*. Here the processes and phenomena are collected taking place in the system relevant to the modeling goal, such as operating units, balance volumes, physical and chemical laws, etc.

3. *Evaluate the problem data*. The a priori known data and parameter values are investigated here that are used in the model. This step contains the investigation what data of the system are measurable and uniquely determines the model inputs and outputs based on the modeling goal and the measurements.

4. *Construct the model equations*. The model equations are developed that can be either differential or algebraic ones.

5. *Solve the models*. A solution procedure is found and implemented for the model equations.

6. *Verify the solution*. We determine whether the model behaves correctly. Model verification includes syntax checking and semantics checking,

as well as the well-posedness checking of the model in mathematical sense, and analysis of computational and dynamic properties.

7. *Calibrate and validate the model*. We estimate the unknown parts of the model from measurements (calibration) and check the quality of the resultant model against independent observation or assumption (validation). The validation can be performed by e.g. comparing the model behavior with the system behavior and/or comparing the model directly with the data. The validation results indicate that the developed model is proper or how to improve it.

This general model development procedure can be applied to develop mathematical model for any kind of physical systems. However, this procedure should be extended or modified a little if the required model has special properties, such as inherent multi-scale nature. We have used a modified version of the seven-step modeling procedure to develop a biomechanical, multi-scale arm model for diagnostic purposes [O3,O6].

2.2 The complexity of dynamic models

Minimal representations are known to have no redundant elements. Therefore, a good model should be minimal based on its performance, size and other measures.

Models are called *functional equivalent models* if all of them satisfy the same modeling goal [3]. Other definition is that two models are *equivalent* if they give rise to the same input-output behavior from the modeling goal point of view.

If one wants to compare functionally equivalent models with respect to their simplicity, a suitable quality or size norm that reflects simplicity should be first defined. One can define integer-valued indices which characterize the general size of a set of functionally equivalent processes, i.e. the *generalized size index* assigns an integer to each model. These could be the dimension of the state variable, the model complexity measure or nonlinearity measure, the relative degree of the model, the dimension of the controllability subspace or distribution, etc.

Several different size indices could be defined for the models that are collected in a vector. In this case the *size norm* is defined as a vector norm of the vector of size indices. Based on the notion of size norm, one of the models is "smaller" or more simple than the another one if its size norm is less than the size norm of the another one.

Therefore, based on the ordering of the functionally equivalent models a model is called *minimal* in this generalized sense, if its size norm is the minimal among the size norms of the other functionally equivalent models [3].

In this thesis the simplicity of the model, i.e. its size norm, is measured the number of state variables and by some kind of measure of nonlinearity, i.e. we use the word "minimal" from an engineering point of view.

The most effective way of focusing on a part of a dynamic system relevant to our purposes is to apply model reduction or model simplification techniques. Minimal models in the generalized sense can be constructed by two methods:

- Iterative model reduction. One iteratively reduces the number of state variables as far as the accuracy of the reduced model satisfies the modeling goal and the reduced model becomes the minimal one.

- Constructing composite models from minimal elements. Using system analysis the main operating units of the system are determined that influence the system dynamics from the aspect of the modeling goal. Then the processes and mechanisms of each operating unit are determined that play important role in the system behavior (from the point of view of the modeling goal). Finally, the mathematical models of the determined mechanisms and processes of the operating units are constructed.

  If the overall model does not satisfy the modeling goal then the model can be extended by additional elements that are originally neglected.

2.3 Identifiability

Identifiability concerns uniqueness of the model parameters determined from input-output data, under ideal conditions of noise-free observations and error-free model structure. Identifiability is a fundamental prerequisite for model identification (model calibration) and qualitative experimental design.

Several approaches for identifiability analysis of non-linear models have appeared in the literature: the local state isomorphism theorem, methods that are based on the linearization procedure, or the power series expansion [4]. Recently differential algebra tools have been applied to study identifiability of nonlinear systems (nonlinearity appears as a polynomial or a rational function in the right side of the state equations) [4, 5]. These methods all exploit the characteristic set of the differential ideal associated with the dynamic equations of the system.

However, problems can arise in testing identifiability for systems started at given initial conditions. In order to guarantee the correctness of the identifiability test based on a characteristic set, one has to check that some structural conditions hold, which are related to the specific initial condition. A natural structural condition which guarantees the validity of the identifiability test is the accessibility of the system from the given initial condition [4, 5].

2.4 Model calibration

The model calibration plays an important role in the seven-step modeling procedure [6] influencing more steps and it may generate a new iteration during the model building.

We often have an incomplete model after the first four steps of the seven-step modeling procedure [1]. We want to obtain these model parameters using experimental data. Because measured data contain measurement errors we can only estimate the unknown or partially known model parameters. This sub-step is called *model calibration*.

The sub-steps of model calibration are [1] the followings.

1. *Analysis of model specification.* Sensitivity analysis with respect to model parameters is performed here to investigate the effect of their changes on the model output and behavior. This parametric sensitivity assessment is performed on the parameters with partially-known and unknown values.

2. *Resampling of measured data*, if it is needed.

3. *Data analysis and preprocessing.* The quality of the estimates depends critically on the quality of the measurement data. Harmful deviations in the data might take the following forms: data with bias, gross error, poor sampling, outliers, jumps, trends, measurement errors, etc. Data screening methods are applied to check the measured data quality.

4. *Model parameter estimation.* The model parameter estimation problem statement is the following [1].
   A parametrized explicit system model is *given* in the form $y^{(M)} = F(x, p^{(M)})$ with the model parameters $p^{(M)} \in \Re^{\nu}$ being unknown, the vector-valued independent variable $x \in \Re^n$ and vector-valued dependent variable $y^{(M)} \in \Re^{\mu}$. A set of measured data and a suitable signal norm are also *given*. Signal norm measures the difference between the model output $y^{(M)}$ and the measured independent variables y to obtain the loss function of the

estimation $L(p) = \|y - y^{(M)}\|$. *Compute* an estimate $\hat{P}^{(M)}$ of $p^{(M)}$ such that $L(p)$ is minimal!

The Nelder-Mead simplex method [7] is one of the most popular optimization methods applied for parameter estimation for nonlinear models. It is a heuristic method, therefore it is important that the initial parameter vector is close to the global minima. The reason for its popularity is that it does not need any analytic or numeric gradient input information of the particular function.

5. *Evaluation of the quality of the estimate.* The confidence intervals of the estimated parameters give information about the quality of the estimates. In the case of linear-in-parameter systems, the covariance matrix of the estimate contains information about the confidence intervals [6]. The covariance matrix can be computed with the least squares method [6].

   In case of the nonlinear parameter estimation we can only apply an approximative approach if we want to estimate the parameter confidence intervals for the estimated coefficient [1]. This approach requires us to depict the error function ($e(p)$) as a function of the parameter p to be estimated. Let e_{opt} be the minimal value of the error function. Then the value of the error function corresponding to the α confidence level can be computed using [1]:

$$e_\alpha = e_{opt}\left(1 + \frac{v}{k-v}F^{-1}(v, k-v, 1-\alpha)\right)$$

   where k is the number of measurements (data points), v is the number of estimated parameters and $F^{-1}(v, k-v, 1-\alpha)$ is the inverse Fisher distribution value for degree of freedom $(v, k-v)$ and confidence level α. The ends of the confidence interval of the estimated parameter can be defined as the abscissas of the error function where the value of the error function is equal to e_α.

   We can obtain information from the shape of the contour plots of the error function, too. The estimation is of good quality if this function has got unique minimum in the value of estimated parameters and the shape of contour plot is approximately circular. The more elliptic the shape of the contour plot (i.e. there is a valley in the error function) is, the more unreliable the estimated values are. In this case the width of the valley gives us information about the accuracy. The wider the valley the lower the accuracy.

2.5 Fault modeling and analysis

Faults generally appear as discrete events in the mathematical models because they have discrete nature, i.e. a fault occurs or does not occur. However the mathematical model of a physical system is continuous in time in most of the cases. Therefore, a mathematical model extended with faults is generally a hybrid-type model.

Nuclear power plants are highly safety-critical and complex systems where the verification and validation of the safety procedures are of great importance. Because of the large number of variables and the complexity of the plant and its dynamical behavior, however, one needs to apply formal methods for this task. At the same time, the dynamics of a nuclear power plant is hybrid in nature caused by the state dependent switching modes and by the discrete control and the safety procedures themselves, therefore the methodology and tools for hybrid systems should be applied.

The need to apply formal verification methods for safety systems in safety-critical areas have long been recognized [8]. However, the majority of the safety-critical industrial studies do not consider dynamical information for the formal analysis, but restrict themselves to hazard and operability analysis (HAZOP) and/or fault mode effect analysis (FMEA) methods extended with stochastic risk assessment information, see e.g. [9, 10].

From the methodological aspect, there are two entirely different approaches to describe and analyze hybrid systems from formal verification point of view. One way is to embed the discrete valued time-dependent variables into an existing dynamical model [11], for example into a state-space model. The other way is to extend the discrete event system techniques [12] with the continuous dynamical information in the form of waiting or execution times to get a timed automaton or Petri net in the simplest case [13], or to define some more or less simple dynamics associated to each state and/or state transition. Driven by the actual aim of modeling, analysis and/or control, further approximations can be or should be made to transform the description to a homogenous discrete event system model form [14]. This allows using, for example, the well-established methods for model analysis developed for discrete event systems.

In our case the coloured Petri nets (CPNs) [15, 16] were chosen as the applied formal verification method.

3 Modeling and model analysis application in a nuclear power plant

3.1 Primary circuit of a nuclear power plant

A nuclear power plant is a complex system because a great number of different processes take place [2, 17] such as thermo-nuclear process, liquid and vapor flow, heat transfer, evaporation, electricity generation, cooling, etc.

One of the most important parts of a nuclear power plant is the primary circuit. The reactor is the main operating unit in the primary circuit that acts primarily as an energy source. The controlled thermo-nuclear processes take place in the reactor. The liquid in the tubes of the primary circuit including the liquid in the reactor, in the primary side tubes of the steam generators and in the pressurizer is circulated by a high speed, and it is under high pressure in order to avoid boiling. The energy generated in the reactor is transferred by the liquid in the primary circuit to the liquid in the steam generator making it boiling. It means that the six steam generators transfer the energy generated by the reactor to the secondary steam flow. The generated secondary circuit vapor is then transferred to the turbines. The pressurizer regulates the pressure in the primary circuit by heating its water content and serves as an indicator for the primary circuit inventory controller by its water level.

3.2 Model development of the primary circuit

The minimal primary circuit model has been constructed from minimal elements based on first engineering principles, i.e. the model has been constructed based on the important conservation balances for conserved extensive quantities such as mass, internal energy, the number of neutrons, supplemented with algebraic constitutive equations. To get a suitable model form for controller design, the system of equations have been transformed into state-space form applying intensive variables. The resulted dynamic model is hybrid and nonlinear in its parameters.

The uniqueness of the model is that it describes all of the important dynamics in the primary circuit using as few elements as possible to design controllers of the operating units and a supervisor controller.

The domain of the model includes the dynamic behavior in normal operating mode together with the load changes between the day and the night periods not including failures and faulty mode transitions.

The model has been realized in MATLAB/SIMULINK environment.

3.3 Model calibration of the primary circuit model

The estimation procedure has to satisfy the constraints so that the estimated values are in the corresponding reliability domains what is constructed based on the thermodynamic and the nuclear power plant operational knowledge.

The identifiability analysis of the model containing initial conditions are investigated using a method based on differential algebra. The results have showed that the model is identifiable.

The model could be decomposed before the model calibration to make it easier. The parameters of the reactor dynamics could be estimated independently of the parameters of the other operating units, thus the reactor forms an independent component of the model. Then the dynamics of the liquid in the primary circuit formed another component that uses the reactor power and temperature in the steam generator as its 'virtual input'. The dynamics of the liquid in the steam generator formes another component that depends on the reactor power and on the temperature of the liquid in the primary circuit. Finally, the fourth component was the pressurizer that depended on the dynamics of the liquid in the primary circuit.

Measured data from three of the VVER-440 units of the Paks Nuclear Power Plant were collected for parameter estimation purposes. The measured data showed the increasing and decreasing of the power of the units when shifting from day to night load conditions and back.

The steps of model calibration were followed. The parameter estimation has been carried out sequentially and component-wise following the dependencies outlined above. An optimization-based parameter estimation method, the Nelder-Mead simplex method [7] was used. For error value we measured the fit in terms of the 2-norm between the measured and the model-predicted output signals.

The quality of estimates has been investigated by the covariance matrix of the estimates when the model was linear in their estimates and by the analysis of the error function of the estimates when the model was nonlinear or hybrid. Linear relationships have been found between the estimated parameters.

3.4 Fault modeling in the primary circuit model

The *PRImary-to-SEcondary leaking* (PRISE) safety procedure [P5,P6], specified by the Paks Nuclear Power Plant personnel, controls the draining of the contaminated water in a faulty steam generator when a primary to secondary circuit non-compensable leaking occurs. A simple low dimensional nonlinear dynamic model of the primary circuit in the Paks Nuclear Power Plant being a VVER-type nuclear power plant together with its relevant safety procedures describing all of the major leaking type faults is developed. The result model is able to simulate the sequence of events of faults and the timing between them. This model is applied to achieve the model based verification of a PRISE safety procedure what is recommended by the experts of the nuclear power plant. The engineering model belongs to a concentrated parameter hybrid model class since the faults are presented as discrete events.

4 New scientific results

The main scientific contributions of the dissertation are summarized in the following thesis points.

Thesis 1. *Model of the primary circuit of a nuclear power plant.* A nonlinear, hybrid and minimal (in a generalized sense) model of the primary circuit of Paks nuclear power plant for controller design purposes has been developed based on first engineering principles. The parts of the model have physical meaning. The model has been built up from minimal elements.

The unique feature of the model is that it describes all of the important dynamics in the primary circuit using as few elements as possible to design controllers of the operating units and a supervisor controller.
(**[P1,P2]**)

1. The minimal, required elements of the real physical system with their connections have been identified. The operating units and their balance volumes have been defined based on them.
2. The model equations have been developed based on first engineering principles (conservation principles).
3. The model equations have been transformed into a form containing intensive variables. Then, the model equations have been transformed into state-space form since it is required for model parameter estimation and controller design.
4. The simulator of the primary circuit has been realized in MATLAB/SIMULINK environment.

Thesis 2. *Model calibration of the primary circuit model.* Model calibration of the primary circuit model has been performed. The nonlinear Nelder-Mead simplex optimization algorithm has been applied since the model is nonlinear in its parameters. An important constraint was that the estimated values had to be in their a priori known reliability domains. The quality of the estimates has also been investigated.
(**[P1,P2,P3,P4]**)

1. The identifiability analysis of the model equipped with given initial conditions has been performed using a method based on differential algebra. The model has been found identifiable.

2. It has been shown that the model can be decomposed based on the operating units and the connections between their dynamics. The model calibration has been performed separately on the decomposed parts.
3. It has been shown that the estimated values show good agreements with their reliability domains.
4. The quality of estimates has been evaluated applying the covariance matrix computed with the least squares method in case of the liquid in the primary circuit and the steam generator. The quality of estimates has been evaluated applying the analysis of the error function in case of the reactor and the pressurizer. Linear relationships have been found between some of the estimated parameters.
5. The integrated model satisfies engineering expectations in the temperatures (except for the temperature of the pressurizer) and the neutron flux and meets not only the qualitative but also the quantitative requirements in both the steady-state values and in the approximate time constants.

Thesis 3. *Primary circuit model with fault modeling*: The primary circuit model has been extended with fault processes modeled by discrete events. The model focuses on the sequence of fault events and does not describe the precise dynamics of energy transportation. The developed model has been found to be suitable for performing the formal verification of the PRISE safety procedure recommended by the experts at Paks Nuclear Power Plant.
(**[P5,P6]**)

1. The dynamic primary circuit model has been extended with fault operations having similar consequences as the PRISE.
2. The faults are modeled by discrete events and represented by indicator variables, therefore the overall model is a hybrid type model.
3. The resulting model is able to simulate the sequence of fault events and the timing between them.
4. The overall model has been successfully used for model-based verification of the PRISE procedure by using the coloured Petri net representation of the overall system model.

A similar model development procedure and iterative model reduction technique were applied to create a multi-scale arm model for diagnostic purposes [O3,O6].

Publications

Publications related to the thesis

[P1] Cs. Fazekas, G. Szederkényi, K. M. Hangos, "A Simple Dynamic Model of the Primary Circuit in VVER Plants for Controller Design Purposes", *Nuclear Engineering and Design*, **237**(10):1071-1087, 2007. (**Thesis 1 and 2**)
Impact factor: 0.461 (2006)

[P2] Cs. Fazekas, G. Szederkényi, K. M. Hangos, "Model Identification of the Primary Circuit at the Paks Nuclear Power Plant", in *Proceedings of The 26th IASTED International Conference on Modelling, Identification, and Control, MIC 2007, pp:464-469, Innsbruck, Austria*, 12-14, February, 2007. on CD. (**Thesis 1 and 2**)

[P3] Cs. Fazekas, G. Szederkényi, K. M. Hangos, "Parameter estimation of a simple primary circuit model of a VVER plant", *IEEE Transaction on Nuclear Science*, Accepted with "revision", 2008. (**Thesis 2**)

[P4] Cs. Fazekas, G. Szederkényi, K. M. Hangos, "Identification of the primary circuit dynamics in a pressurized water nuclear power plant", *17th IFAC Word Congress, Seoul, Korea*, 6-11, July, 2008. (**Thesis 2**)

[P5] E. Németh, T. Bartha, Cs. Fazekas, K.M. Hangos, "Verificarion of a primary-to-secondary leaking safety procedure in a nuclear power plant using coloured Petri nets", *Reliability Engineering and System Safety*, 2007, Accepted with "revision". (**Thesis 3**)

[P6] E. Németh, Cs. Fazekas, G. Szederkényi, K. M. Hangos, "Modeling and simulation of the primary circuit of the Paks Nuclear Power Plant for control and diagnosis", in *Proceedings of The 6th European Simulation and Modelling, EuroSim 2007, Ljubljana, Slovenia*, 9-13, September, 2007. on CD. (**Thesis 3**)

Other publications

Other publications not connected to the topic of this thesis are as follows:

[O1] Cs. Fazekas and K. M. Hangos, "Model Building, Verification and Sensitivity Analysis of a Multi-Scale Limb Model", in *Proceedings of The 5th International PhD Workshop on Systems and Control - Young Generation Viewpoint, Balatonfüred, Hungary*, 2004. on CD.

[O2] Cs. Fazekas, Gy. Kozmann, K. M. Hangos, "Hierarchical Modelling in Biology: a Systematic Build-Up of a Limb Model", Technical report of the Systems and Control Laboratory SCL-003/2004, Computer and Automation Research Institute of HAS, 2004. `http://daedalus.scl.sztaki.hu`.

[O3] Cs. Fazekas, Gy. Kozmann, K. M. Hangos, "Hierarchical Modelling in Biology: Systematic Building of Limb Models", *IFAC Word Congress, Prague, Czech Republic*, 3-8 June 2005. on DVD. ISBN: 0-08-045108-X.

[O4] Cs. Fazekas and K. M. Hangos, "Experimental Design for Parameter Estimation of a Multi-Scale Arm Model", in *Proceedings of The 6th International PhD Workshop on Systems and Control - Young Generation Viewpoint, Izola-Simonov zaliv, Slovenia*, October 4-8, 2005. on CD.

[O5] Cs. Fazekas, Gy. Kozmann, K. M. Hangos, "Biomechanikai rendszerek többléptékű modellezése", *Információ és Menedzsment az Egészségügyben (IME)*, 5(3):45-48, 2006.

[O6] Cs. Fazekas, Gy. Kozmann, K. M. Hangos, "Multi-scale Modeling and Time-scale Analysis of a Human Limb", *Multiscale Modelling and Simulation*, 6(3):761-791, 2007. ***Impact factor: 1.736 (2005)***

[O7] Cs. Fazekas, Gy. Kozmann, T Magos, K.M. Hangos, "Parameter Estimation of a Simple Hierarchical Arm Model", Technical Report of the Systems and Control Laboratory, SCL-002/2007, `http://daedalus.scl.sztaki.hu`.

[O8] Cs. Fazekas, D. Csercsik, G. Szederkényi, K. M. Hangos, "Simulator for multi-scale musculoskeletal models with reflex circuits", *Proceedings of the 6th European Simulation and Modelling Conference, EuroSim 2007*, Ljubljana, Slovenia, 9-13, September, 2007

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