Veszprémi Egyetem
Számítástudomány Alkalmazása Tanszék
Műszaki Informatika Szak

DIPLOMADOLGOZAT

Asymptotic Stability of an Evaporator System

Pongrácz Barna

2001

Veszprémi Egyetem
Számítástudomány Alkalmazása Tanszék
Műszaki Informatika Szak

DIPLOMADOLGOZAT

Asymptotic Stability of an Evaporator System

Pongrácz Barna

Témavezető: Dr. Hangos Katalin

2001

Nyilatkozat

Alulírott Pongrácz Barna, diplomázó hallgató, kijelentem, hogy a diplomadolgozatot a Veszprémi Egyetem Számítástudomány Alkalmazása tanszékén készítettem mérnök-informatikus diploma (master of engineering in information technology) megszerzése érdekében.

Kijelentem, hogy a diplomadolgozatban foglaltak saját munkám eredményei, és csak a megadott forrásokat (szakirodalom, eszközök, stb.) használtam fel.

Tudomásul veszem, hogy a diplomadolgozatban foglalt eredményeket a Veszprémi Egyetem, valamint a feladatot kiíró szervezeti egység saját céljaira szabadon felhasználhatja.

Veszprém, 2001. május 3.

Pongrácz Barna

Köszönetnyilvánítás

Legelőször témavezetőmnek, Dr. Hangos Katalinnak szeretnék köszönetet mondani azért a lelkiismeretes segítségért és odafigyelésért, amivel az utóbbi két évben munkámat kísérte. Köszönettel tartozom Édesapámnak, akinek barátsága sokat jelent a számomra. Köszönet illeti Szederkényi Gábort, és mindazokat, akik segítették eme diplomadolgozat megszületését.

Summary

The subject of this diploma work is the investigation of dynamic properties of process systems given in the form of differential and algebraic (DAE) set of equations. My task was to investigate the asymptotic stability of systems given in DAE form on the example of a two-phase lumped parameter evaporator system. Since the general methods of checking stability can only be applied to purely differential models, we substitute the algebraic equations into the differential ones. With the help of structure matrices I found that there are cases when the algebraic variables cannot be expressed from the algebraic equations. The variables causing problem can be identified, and must be transformed into differential ones to derive a model in state space form. I applied this method to the evaporator model: According to the structure matrix of the algebraic equations, five problematic variables were found. The five relevant equations were differentiated by time, therefore the other part of algebraic equations became substitutable into the differential ones. This way I derived a state space representation consisting of nine differential equations which was suitable for stability analysis.

The analysis of asymptotic stability was performed using contraction technique, which gives rise to investigate stability with substituting the values of possible operating points.

I prepared the Simulink model of the evaporator system in MATLAB environment. For simulations, I used a simplified (substitutable) model of the evaporator system for which an operating point had to be found. The model had no unique operating point since the equation system determining the operating point was under- and over-determined. Therefore I have changed the natural specification and gave the values of some state variables instead of some input variables. This way the operating point became unique.

In the numerical model above I completed the investigation of asymptotic stability of the given operating point with the help of a script written in Maple. For this I used the theoretical results of contraction analysis: I investigated the eigenvalues of the Jacobian of the model in the operating point. I applied this method for the two different models derived from eliminating, or differentiating the algebraic equations. This way I came to the consequence that the eigenvalues of these two representations

are identical, apart from the appropriate number of zero eigenvalues caused by the difference on the size of these models. (The evaporator model given by substitution consists of four, the other derived from differentiation consists of seven differential equations.)

I analyzed these methods and investigated their applicability to other models given in the form of DAE.

Keywords: *DAE models, structural analysis, differential index, asymptotic stability, contraction technique.*

Tartalmi összefoglaló

Diplomamunkám témája a differenciál-algebrai (DAE) egyenletrendszer formájában adott folyamatmodellek jellemzö tulajdonságainak vizsgálata. Feladatom az, hogy egy koncentrált paraméterű kétfázisú elpárologtató rendszer nemlineáris modelljének példáján DAE egyenletrendszerrel adott modellű dinamikus rendszerek aszimptotikus stabilitását vizsgáljam.

Mivel az általános stabilitásvizsgálati módszerek tisztán differenciális modellekre alkalmazhatók, az algebrai egyenleteket rendszerint behelyettesítjük a differenciálegyenletekbe. Struktúramátrixok felírásával megállapítottam, hogy az algebrai változók nem minden esetben fejezhetők ki az algebrai egyenletekből, azaz nem mindig tudjuk az algebrai egyenleteket behelyettesíteni a differenciálegyenletekbe. Kiválaszthatók azok a változók, amelyeket differenciális változókká kell alakítani, hogy állapottér modell alakjára hozzuk a modellt. Ezt az elpárologtató rendszer példáján úgy hajtottam végre, hogy a struktúramátrix alapján - öt algebrai változót differenciális változóvá alakítottam a megfelelő öt algebrai egyenlet idő szerinti deriválásával. Így a maradék algebrai egyenletek már behelyettesíthetővé váltak. Ezzel a módszerrel az adott példában egy kilenc differenciálegyenletből álló egyenletrendszert kaptam, amely már alkalmas a stabilitás vizsgálatára.

A stabilitásvizsgálatot kontrakciós technikával végeztem el, amely formulába a lehetséges munkapontok adatait behelyettesítve a stabilitás megvizsgálható.

Elkészítettem a rendszer Simulink modelljét (MATLAB környezetben).
A szimulációs vizsgálathoz egy egyszerűsített (behelyettesíthető) modellt használtam, amelyhez munkaponti értékeket kellett találnom. A modellnek nem volt egyértelmű munkapontja, mivel szimulációhoz szükséges munkapontot meghatározó egyenletrendszer alulhatározott volt a differenciális, és túlhatározott az input változók szempontjából. Ezért megváltoztattam a természetes specifikációt, és bizonyos input változók helyett állapotváltozók értékeit adtam meg, így a munkapont többi része már egyértelművé vált.

A fenti numerikus modellen egy általam írott Maple script segítségével elvégeztem a kapott munkapont stabilitásának vizsgálatát. Ehhez a kontrakciós analízis eredményeit használtam fel: A modell munkaponti Jakobi mátrixának sajátértékeit vizsgáltam. Ezt alkalmaztam az algebrai egyenletek behelyettesítésével; valamint az algeb-

rai egyenletek differenciálásával kapott két különböző modellre. Megállapítottam, hogy a két reprezentáció sajátértékei megegyeznek, elegendő számú nulla sajátértékkel kiegészítve (Az elpárologtató egyik modellje négy, a másik hét differenciálegyenletből áll).

A kapott módszereket elemeztem, és vizsgáltam azok alkalmazhatóságát más DAE formában adott modellekre.

Kulcsszavak: *DAE modell, strukturális analysis, differenciális index, aszimptotikus stabilitás, kontrakciós technika.*

Contents

1 Introduction **3**

1.1 Analysis of task specification 3

1.2 Literature review 5

1.3 The evaporator system 6

2 Dynamic models in DAE form **7**

2.1 Model equation of the evaporator 8

2.1.1 Balance equations 8

2.1.2 Transfer rate equations 8

2.1.3 Algebraic equations 8

2.1.4 Variables and constants 9

2.2 The structure of DAE models 10

2.3 The structure matrix 11

2.4 Qualitative properties of DAE 13

3 Transformation of DAE **15**

3.1 The transformation method 15

3.2 Transformation of the evaporator model 15

3.3 The transformed model of the evaporator 18

3.3.1 Differential equations 18

3.3.2 The transformed variables 19

4 Model analysis: stability **20**

4.1 Stability analysis basics 20

4.1.1 Contraction technique 21

4.1.2 Lyapunov technique 21

4.2 Stability analysis of the evaporator 22

4.2.1 Application of contraction technique 24

4.2.2 Application of Lyapunov technique 25

5 Simulations **27**

5.1 The evaporator model used in simulations 27

5.2 The SIMULINK model of the evaporator 28

5.3 Steady-state operating points of the evaporator 29
5.4 Simulation results 32

6 Conclusion and future work **38**

List of Figures

1 Block scheme of the evaporator system 7
2 The Simulink model of the evaporator system 30
3 Simulation 1.1. Different initial conditions 34
4 Simulation 1.2. Different initial conditions 35
5 Simulation 2. Lack of steady state 36
6 Simulation 3. Unique operating point 37

List of Tables

1 Structure matrix 12
2 Triangular structure matrix 12
3 Another example: Square in structure 12
4 Structure matrix of algebraic equations I. 16
5 Structure matrix of algebraic equations II. 16
6 The reduced structure matrix 17
7 Eigenvalues of the two models for different operating points. 25
8 Table of Constants 28
9 Singular algebraic equation set for computing operating points 31
10 Operating points for different values of specification 32

1 Introduction

1.1 Analysis of task specification

The stability investigation of process systems plays an important role in not just the chemical, petroleum and related industries, but in the area of environmental protection. One important problem for research is the question of asymptotic stability, where we examine the change of extensive (mass and internal energy of phases) and intensive (temperature) quantities near an operating point.

Since input-output models are not able to describe the internal states as the "memory" of the system, process systems are usually represented by a state-space model description [2]. This consists of two equations: The state equation is a set of first order differential equations where the differential variables are the states of the system. The change of states depends on the state and the input variables of the system. The output equation is a set of algebraic equations where the outputs are determined from the inputs and the states.

Depending on the form of these equations, a state-space representation can be linear or nonlinear. Linear description is simple and enables an easy way to investigate system properties, though nonlinear models describe the physical system much more properly. In this work we use nonlinear models.

Asymptotic stability means whether the state variables of the system return to their steady state after small diversions caused by external disturbances. In contrast to the linear case, where the complete system is called asymptotically stable, in nonlinear systems asymptotic stability is a property of an operating point.

The mathematical model of a process system consists of differential equations derived from first engineering principles (balance equations), and sufficient number of algebraic (constitutive) equations which determine relationship between the differential and algebraic variables. These relations are not always given in explicit form but computed by subroutines of special program packages. This kind of description is called differential algebraic equation set (DAE). These systems are hard to investigate, so we usually try to transform them into a set of ordinary differential equations (ODE form). Sometimes the algebraic equations cannot be substituted into the balance equations because of their singularity. It's a pity because general methods for investigating asymptotic stability are only given for ODE systems!

A typical example for a simple but hard-to-investigate class of process systems is a lumped parameter evaporator system of two phases with one physical input (liquid) and two physical outputs (vapour,liquid). The dynamic model of the system is given in DAE form. We want to analyze asymptotic stability of an operating point of the system.

With the help of structure matrices it is shown that the algebraic variables cannot be expressed from the algebraic equations and substituted into the differential ones because of the multiple relations and the nonlinearity. As stability investigation methods can only be applied for pure differential models, we want to find a way for transforming the DAE model into ODE form.

Applying a simple two-step algorithm, a state-space representation of nine differential equations is derived, so we are given a purely differential model form. Using the results of constraction analysis and the Lyapunov technique we were searching for the answer to the question of asymptotic stability. At the end of this work several interesting stable/instable cases are shown by simulations performed with Matlab's Simulink package.

The outline of this work is as follows:
In this report asymptotic stability of a two phase evaporator system is investigated. After the system description (Chapter 1), the model equations from first engineering principles are established in DAE form (Chapter 2).

Chapter 3 an algorithm using structure matrices is introduced to find a way for eliminating the algebraic equations. The method provides five non-substitutable algebraic equations, which are transformed by means of differentiation. That leads to a system of ordinary differential equations (ODEs).

In Chapter 4 the basics of stability analysis is settled, the Lyapunov-technique and the results of contraction analysis are presented, giving rise to the chance of analyzing asymptotic stability on our system represented in two different forms. As an additional result, a connection is found between these two representations while applying contraction technique.

Chapter 5 contains numerical simulations which are implemented in Matlab's Simulink. The operating point of the system is given by using Maple. Several salutary examples are shown here.

In Chapter 6 the given results and conclusions are summarized, and the directions

of future research are pointed out.

In the Appendix, the source code of scripts used are placed.

1.2 Literature review

In the general case the mathematical description of lumped process systems is given in differential algebraic equation (DAE) form [4] consisting of differential (conservation balance) equations and algebraic (constitutive) equations. The dynamical behaviour of a system given in DAE form is not easy to investigate by standard methods because the algebraic variables cannot be expressed from the algebraic equations in some cases.

The non-substitutable part of the constitutive algebraic equations can be transformed into differential ones by differentiation [4]. After that we can eliminate algebraic variables and get to a purely differential equation system which describes the dynamics properly. he solvability of algebraic equations (which means that we can fully eliminate them) depends on their structure [4]. A DAE set of equations has differential index 1, if and only if the algebraic part of the set is structurally solvable with respect to the algebraic variables. The related notions and relations can be found in Chapter 2.4. In case of nonlinear equations solvability is made difficult by the presence of the same set of variables in a set of equations, called blocks. The structure of a DAE system can be investigated with structure matrices or equation-variable graphs [7].

For purely differential models, we have standard tools for stability analysis because the state equation of finite dimensional systems is a set of 1st order explicit differential equations [3].

In case of linear time invariant case the state equation is given in the form of

$$\dot{x}(t) = Ax(t) + Bu(t)$$

where x is the state vector, u is the input vector and A, B are matrices of the appropriate dimensions. We call a LTI system asymptotically stable if the solution of the equation

$$\frac{dx}{dt} = Ax,\ x(0) \neq 0$$

converges to zero as time goes to the infinity. It is known that if the eigenvalues of the

state matrix A have uniformly negative real parts then the system is asymptotically stable [2].

In nonlinear case we consider systems with the state equation given in a special *input-affin* form:

$$\dot{x}(t) = f(x(t)) + \sum_{i=1}^{m} g_i(x(t))u_i(t))$$

where $x(t)$ and $u_i(t)$ are vectors, f and g_i are smooth nonlinear functions [3].

There are two basic tools for stability analysis for models given in input-affin form: The *contraction technique* is based on the contractive property of function f. If the Jacobian of f has negative eigenvalues in the steady state, then f is contractive, and stability is proved [5]. *Lyapunov technique* uses a generalized energy function which is positive definite and dissipative (its time-derivative is descending) [3]. A special way of Lyapunov analysis is described in [6], showing a way of passivity based control design for single input-single output systems.

1.3 The evaporator system

Let us consider an evaporator system with two phases (liquid and vapour) with respective holdups M_L and M_V, internal energies as U_L and U_V and temperatures as T_L and T_V . Liquid is fed into the vessel and vapourized by a heating stream. Liquid and vapour are taken from the system as depicted in Fig.1.

The inflow rate of water (F), the outflow rates of liquid (L) and vapour (V) and the energy input flowrate (Q) are not determined that is they are regarded as potential input variables. The liquid-to-vapour flowrates of mass and energy is denoted by E and Q_E. For describing dynamic behaviour we use a lumped parameter model; both phases are regarded perfectly stirred. Pressure can change during the process, and - in the general model - the physico-chemical properties are considered as functions of other variables - so they are not constants. The system is controlled by the input variables.

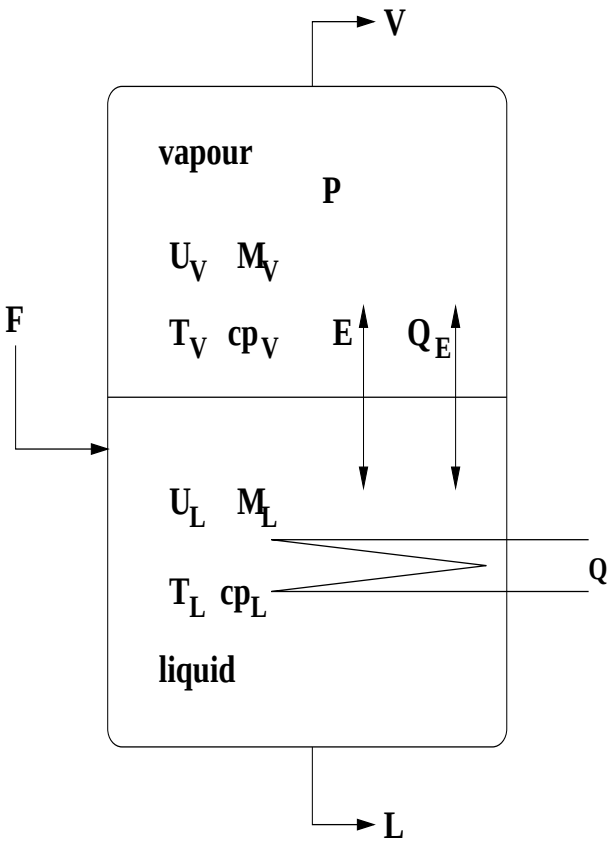

Figure 1: Block scheme of the evaporator system

2 Dynamic process models in DAE form

The basic equations of dynamic process models are differential equations which characterize the dynamics of the system. We call them conservation balances because they are constructed for conservative extensive quantities such as mass and internal energy. In an equation like that we describe the change of a conservative extensive variable using its time-derivative so we get to differential equations. Therefore conservative variables will be the differential variables in the DAE model [1].

Other variables also occur in these equations which are called algebraic or constitutive variables and need to be described by algebraic dependencies. These equations are called algebraic or constitutive equations.

2.1 Model equations of the evaporator system

Since we have two balance volumes they generate four conservation balances - one for mass and one for energy in both phases [1]:

2.1.1 Balance equations

(*Mass balance,liquid:*)

$$\frac{dM_L}{dt} = F - E - L \tag{1}$$

(*Mass balance,vapour:*)

$$\frac{dM_V}{dt} = E - V \tag{2}$$

(*Energy balance,liquid:*)

$$\frac{dU_L}{dt} = Fh_F - Eh_{LV} - Lh_L + Q - Q_E \tag{3}$$

(*Energy balance,vapour:*)

$$\frac{dU_V}{dt} = Eh_{LV} - Vh_V + Q_E \tag{4}$$

2.1.2 Transfer rate equations

(*Mass transfer:*)

$$E = (k_{LV} - k_{VL})A(P^* - P) \tag{5}$$

(*Energy transfer:*)

$$Q_E = (u_{LV} - u_{VL})A(T_L - T_V) \tag{6}$$

2.1.3 Algebraic equations

$$PV_V = \frac{M_V}{m_\omega}RT_V \tag{7}$$

$$U_V = M_V cp_V T_V \tag{8}$$

$$U_L = M_L cp_L T_L \tag{9}$$

$$cp_V = \mathbf{cp_V}(T_V, P) \tag{10}$$

$$cp_L = \mathbf{cp_L}(T_L, P) \tag{11}$$

$$V_L = \frac{M_L}{\rho_L} \tag{12}$$

$$V_V = V_T - V_L \tag{13}$$

$$P^* = \mathbf{P}^*(T_L) \tag{14}$$

$$\rho_L = \rho_{\mathbf{L}}(T_L, P) \tag{15}$$

$$h_V = \mathbf{h_V}(T_V, P) \tag{16}$$

$$h_L = \mathbf{h_L}(T_L, P) \tag{17}$$

$$h_{LV} = \mathbf{h_{LV}}(T_L, P) \tag{18}$$

$$h_F = \mathbf{h_F}(T_F, P) \tag{19}$$

$$k_{LV} = \mathbf{k_{LV}}(T_L, T_V, P) \tag{20}$$

$$k_{VL} = \mathbf{k_{VL}}(T_L, T_V, P) \tag{21}$$

$$u_{LV} = \mathbf{u_{LV}}(T_L, T_V, P) \tag{22}$$

$$u_{VL} = \mathbf{u_{VL}}(T_L, T_V, P) \tag{23}$$

2.1.4 Variables and constants

Differential variables:

M_L	mass holdup of liquid	M_V	mass holdup of vapour
U_L	internal energy of liquid	U_V	internal energy of vapour

Input variables:

L	liquid flowrate	V	vapour flowrate
F	feed flowrate	Q	energy input flowrate

Transfer rate variables:

E	interphase mass flowrate	Q_E	interphase energy flowrate

Other variables:

P	system pressure	ρ_L	liquid density
V_L	liquid phase volume	V_V	vapour phase volume
cp_L	liquid specific heat capacity	cp_V	vapour specific heat capacity
T_L	temperature of liquid	T_V	temperature of vapour
P^*	vapour pressure	T_F	feed temperature - *disturbance*
h_V	vapour specific enthalpy	h_L	liquid specific enthalpy
h_{LV}	interphase vapour specific enthalpy	h_F	feed specific enthalpy
k_{LV}	liquid-to-vapour heat transfer coef.	k_{VL}	vapour-to-liquid heat transfer coef.

u_{LV}	liquid-to-vapour heat transfer coef.	u_{VL}	vapour-to-liquid heat transfer coef.

System constants are:

A	interfacial area	m_ω	molecular weight
R	universal gas constant	V_T	volume of the vessel

2.2 The structure of DAE models

Our system model derived from first principles is given in DAE form, which consists of differential and algebraic equations [7]:

$$(D) \; : \quad \frac{dx}{dt} = f(x, z_1, z_2) \quad , \quad x(t_0) = x_0 \tag{24}$$

$$(A1) \; : \quad z_1 = g_1(x, z_2) \tag{25}$$

$$(A2) \; : \quad 0 = g_2(x, z_1, z_2) \tag{26}$$

where

x	differential variables
(D)	differential equations (conservation balances)
z_1	algebraic variables of the 1st type
$(A1)$	algebraic equations of the 1st type
z_2	algebraic variables of the 2st type
$(A2)$	algebraic equations of the 2st type

The 1st type of constitutive relations are in explicit form for their algebraic variables z_{1i}. An example for this type is called physico-chemical property equations where the nonlinear function g_1 is usually not known explicitly and/or non-invertible (computed by a subroutine in a package). The algebraic variables z_1 on the left-hand side of these equations are the corresponding physico-chemical property variables. The 2nd type of constitutive equations are inherently implicit, they are determined by other relations.

The DAE form of a process system consisting of conservation balances and constitutive equations is not suitable for dynamic analysis purposes. Therefore we aim at transforming our DAE form into an *input-affin* nonlinear state equation, which consists of a dynamical description of conservative and perhaps other variables and

therefore they form an advantageous kind of description. This transformation is performed by means of elimination, expressing all the algebraic variables and substituting them into the differential part.

Since we have a differential algebraic equation (DAE) model with zero degree of freedom, we can derive a transformed model from it with only differential equations, by means of elimination that is substitution of the algebraic variables into the differential equations. In case of linear algebraic equations this is very simple, but with nonlinear equations it can be hard or even impossible. For investigating the structure of the algebraic part of the model we use a special mathematical tool.

2.3 The structure matrix

The structure matrix of a system of equations is a matrix M with rows associated to equations and columns to variables. If Eq.(i) contains variable x_j then $M_{ij} = [X]$, otherwise $M_{ij} = [\ ]$. To illustrate the usage of structure matrices consider the following set of equations:

$$\begin{aligned} e^{x_1} &= 4 + 1/x_3 \\ 4 + 5t &= -8 + x_3 \\ x_1 x_2 &= 3 + v \end{aligned}$$

Let's solve the equations for x_1, x_2, x_3 !

A simple algorithm provides the result:

(1) Take a row which contains only one unexpressed variable.
(2a) If exists, express the variable from the equation attached, and go back to (1) till you have equations left.
(2b) If there are variables left but none of them is single the algorithm stops with a partial result.

An example for this algorithm is seen in Table 1. At first, we express x_3 from Eq.(2). Since x_3 is given we get x_1 from Eq.(1). Finally, x_2 is from Eq.(3).

We use structure matrices to get a better algorithm: we transform the original matrix into a lower triangular form with simple exchanges of rows and columns. The former example is shown in lower triangular form in Table 2.

	x_1	x_2	x_3
Eq.(1)	**X**		X
Eq.(2)			**X**
Eq.(3)	X	**X**	

Table 1: Structure matrix

	x_3	x_1	x_2
Eq.(2)	**X**		
Eq.(1)	X	**X**	
Eq.(3)	X		**X**

Table 2: Triangular structure matrix

The variable at the diagonal is expressed in every step. It is easy to see that if we can transform the matrix into lower-triangle form we can express and substitute all the variables easily.

Let's see an example when it is not possible! This is the case when we have a matrix with one or more elements above the diagonal.

	y_1	y_2	y_3
Eq.(4)	**X**		
Eq.(5)		***X***	***X***
Eq.(6)	X	***X***	***X***

Table 3: Another example: Square in structure

In Table 3. we can see two equations containing unexpressed variables y_2 and y_3. If we have linear equations the solution of this 2X2 equation block can be done easily, but with nonlinear equations this can be very difficult. In general, troubles are caused by 2X2, 3X3 etc. blocks, "squares" getting across the diagonal which makes computing hard, referring to at least two common variables in a - usually nonlinear - set of equations.

2.4 Qualitative properties of DAE models: solvability and index

In the previous section we established a method for expressing the desired algebraic variables from a set of algebraic equations. But what would assure us of the solvability of these equations? In this section we get acquainted with some notions concerning to the solvability of a DAE model.

The *differential index* is a natural number which shows how many times the algebraic part of a DAE model must be differentiated to get a purely differential model. The differential index is zero if the model contains differential equations only. If we are given a fully expressible (nonsingular) set of algebraic equations we have to differentiate it once, so the differential index equals to one. If the algebraic set of equations have to be differentiated more times, we speak about high-index models [4].

The *degrees of freedom* of a set of equations equals to the difference of the number of equations and the number of variables: $DOF = NUM_{EQU} - NUM_{VAR}$. A solvable DAE has to have zero degrees of freedom both for the differential and the algebraic subset of equations. If we have a system with $DOF_{algebraic} = k > 0$, we have to specify k algebraic variables (determine them as constants). The condition $DOF = 0$ is necessary, but not sufficient; we must take into account another notion about the solvability of the algebraic subset of equations.

The *structural rank* of a set of algebraic equations is the maximal rank of its structure matrix. If it equals to the number of algebraic equations, then we call the model *structurally solvable*. It means that the algebraic set of equations is of full rank regarding to the algebraic variables. If the algebraic equation set is singular, there are under- and over-determined parts of the set, and the algebraic variables are not fully expressible.

The differential index equals to one if and only if the algebraic part of the model is structurally solvable. Thus, if the set of algebraic equations is not structurally solvable, the algebraic variables are not expressible and cannot be substituted into the differential equations, therefore the differential index is more than one. Consequently, DAE models with non-expressible algebraic equations are high-index models.

Note that structural solvability is a "best case" notion and does not imply solvability for all relevant models; in some cases the concrete values in the specification of variables can spoil solvability by making the set of algebraic equations singular.

3 Transformation of the DAE model into state-space model form

In the previous chapter we have determined the DAE model of the evaporator system. As the DAE representation makes the investigation of stability much harder, we try to derive a purely differential mathematical model. This section is concerned with the transformation of our differential-algebraic model form into a purely differential representation to get the desired state-space model.

3.1 The transformation method

We present an optimal way of finding a purely differential equation model. The method uses an index 1 DAE model and consists of two steps:

- Construct the structure matrix of algebraic equations in lower triangular form and determine the set of expressible variables. Eliminate these variables (express and substitute them into the differential equations).
- Differentiate with respect to time the remainder set of equations belonging to non-expressible algebraic variables. These variables will be the new additional differential variables of the derived differential model.

This algorithm gives us a purely differential equation model which is easier to investigate, at the expense of a larger set of equations.

3.2 Transformation of the evaporator model

Our task seems to be simple: we have four state equations and 17 algebraic equations with four state and seventeen algebraic variables, and want to keep only the four state equations with its own variables. Let's express the algebraic variables with the state variables and substitute them into the state equations!

As we are interested in the elimination of the algebraic variables, we have to take into account the dependence of algebraic variables only. The original structure of algebraic equations is seen in Table 4.

We can see that our algorithm in Section 3.1 fails in the first step since there are no variables alone in any rows. The blocks causing troubles connect the variables

	P	V_V	T_V	cp_V	cp_L	T_L	V_L	P^*	ρ_L	h_V	h_L	h_{LV}	h_F	k_{LV}	k_{VL}	u_{LV}	u_{VL}
7	X	X	X														
8			X	X													
9					X	X											
10	X		X	X													
11	X				X	X											
12							X		X								
13		X					X										
14						X		X									
15	X					X			X								
16	X		X							X							
17	X					X					X						
18	X					X						X					
19	X												X				
20	X		X			X								X			
21	X		X			X									X		
22	X		X			X										X	
23	X		X			X											X

Table 4: Structure matrix of algebraic equations I.

	V_V	V_L	ρ_L	P^*	h_V	h_L	h_{LV}	h_F	k_{LV}	k_{VL}	u_{LV}	u_{VL}	P	T_V	cp_V	cp_L	T_L
7	X												**X**	**X**			
8														**X**	**X**		
9																**X**	**X**
10													**X**	**X**	**X**		
11													**X**			**X**	**X**
12		X	X														
13	X	X															
15			X										**X**				**X**
14				X													X
16					X								X	X			
17						X							X				X
18							X						X				X
19								X					X				
20									X				X	X			X
21										X			X	X			X
22											X		X	X			X
23												X	X	X			X

Table 5: Structure matrix of algebraic equations II.

	ρ_L	V_L	V_V	P	T_V	cp_V	cp_L	T_L
15	**X**			X				X
12	X	**X**						
13		X	**X**					
7			X	X	X			
8					X	X		
9							X	X
10				X	X	X		
11				X			X	X

Table 6: The reduced structure matrix

P, T_V, T_L, cp_V and cp_L. In the next step we group them to the right side and separate the 1st and 2nd type of algebraic equations. As a result we have the decomposed situation depicted in Table 5.

It is evident that the physico-chemical property functions can be expressed from only one equation so we just have to deal with equations (7)-(13) and (15). Blocks are between equation pairs (7)-(10) , (8)-(10) , (9)-(11) and (11)-(15). The five equations from (7) to (11) contains five non-expressible variables $(P, T_V, cp_V, T_l, cp_L)$ so we separate them to the bottom. This way we arrive to a reduced 8X8 structure matrix seen in Table 6.

Now it's easy to express ρ_L and V_L to get V_V that will be used later in substitution:

$$V_V = V_T - \frac{M_L}{\rho_L(T_L, P)} \tag{27}$$

The remainder (non-expressible) part contains 5 equations with 5 unexpressed variables in a 5X5 block of the structure matrix (see Table 6.): the down-right block of the reduced structure matrix with variables P, T_V, cp_V, cp_L and T_L. After performing the second step of the algorithm (differentiation by time) on this remainder set, we get a set of first order differential equations. The derived model has 9 differential variables - 5 of them are the consequence of the applied algorithm.

3.3 The transformed state space model of the evaporator system

3.3.1 Differential equations

The representation we obtained by the method in section 3.2 consists of 9 differential equations:

$$\frac{dM_L}{dt} = -kA(P^*(T_L) - P) + \mathbf{F} - \mathbf{L} \tag{28}$$

$$\frac{dM_V}{dt} = kA(P^*(T_L) - P) - \mathbf{V} \tag{29}$$

$$\frac{dU_L}{dt} = -kA(P^*(T_L) - P)h_{LV} - uA(T_L - T_V) - \mathbf{L}h_L + \mathbf{F}h_F + \mathbf{Q} \tag{30}$$

$$\frac{dU_V}{dt} = kA(P^*(T_L) - P)h_{LV} + uA(T_L - T_V) - \mathbf{V}h_V \tag{31}$$

$$\frac{dP}{dt} = \frac{R}{m_\omega}\,(\frac{\frac{dM_V}{dt}T_V\rho_L(P,T_L) + M_V\frac{dT_V}{dt}\rho_L(P,T_L) + M_V T_V\frac{d\rho_L(P,T_L))}{dt}}{V_T\rho_L(P,T_L) - M_L} - \\ -\frac{M_V T_V\rho_L(P,T_L)(V_T\frac{d\rho_L}{dt} - \frac{dM_L}{dt})}{(V_T\rho_L(P,T_L) - M_L)^2}\ ) \tag{32}$$

$$\frac{dT_L}{dt} = \frac{cp_L\ (kA(P^*(T_L) - P)(U_L - h_{LV}M_L) - uA(T_L - T_V)M_L}{(M_L cp_L)^2} + \\ +\frac{M_L(h_F\mathbf{F} - h_L\mathbf{L} + \mathbf{Q}) - U_L(\mathbf{F} - \mathbf{L})\ ) - \frac{dcp_L(P,T_L)}{dt}U_L M_L}{(M_L cp_L)^2} \tag{33}$$

$$\frac{dT_V}{dt} = \frac{cp_V\ (kA(P^*(T_L) - P)(h_{LV}M_V - U_V) + uA(T_L - T_V)M_V}{(M_V cp_V)^2} + \\ +\frac{\mathbf{V}(U_V - h_V M_V)\ ) - \frac{dcp_V(P,T_V)}{dt}U_V M_V}{(M_V cp_V)^2} \tag{34}$$

$$\frac{dcp_L}{dt} = \frac{dcp_L(T_L,P)}{dt} \tag{35}$$

$$\frac{dcp_V}{dt} = \frac{dcp_V(T_V, P)}{dt} \tag{36}$$

where $k = k_{LV}(P, T_L, T_V) - k_{VL}(P, T_L, T_V),\ u = u_{LV}(P, T_L, T_V) - u_{VL}(P, T_L, T_V)$, $h_{LV}(P, T_L),\ h_F(P, T_F),\ h_V(P, T_L)$ are thermodynamic property functions.

Note that equation (27) is used up in substitution and equations (32) to (36) are transformed by the method described above.

3.3.2 The transformed variables

The transformed representation contains the following variables and constants:

Differential variables:

M_L	mass holdup of liquid	M_V	mass holdup of vapour
U_L	internal energy of liquid	U_V	internal energy of vapour
T_L	temperature of liquid	T_V	temperature of vapour
cp_L	liquid specific heat capacity	cp_V	vapour specific heat capacity
P	system pressure		

Input variables:

F	feed flowrate	Q	energy input flowrate
L	liquid flowrate	V	vapour flowrate

System constants are:

A	interfacial area	m_ω	molecular weight
R	universal gas constant	V_T	volume of the vessel

We distinguish the potential input variables present in a natural specification $(\mathbf{F}, \mathbf{L}, \mathbf{V}, \mathbf{Q})$ by boldface typesetting.

4 Model analysis: stability

This chapter deals with notions and techniques for analysing stability. These are then applied to the case of the evaporator system.

4.1 Stability analysis basics [2]

Let us have a truncated nonlinear state equation (with $u(t) = const$) as follows

$$\frac{dx}{dt} = f(x,t) \tag{37}$$

and let it have two solutions:

- $x^0(t)$ for $x^0(t_0)$ as the ordinary solution and
- $x(t)$ for $x(t_0)$ which is a "perturbed solution".

Stability of a solution:

The solution $x^0(t)$ of Eq.(37) is stable if for any given $\epsilon > 0$ there exists a $\delta(\epsilon, k_0)$ such that all solutions with $||x(t_0) - x^0(t_0)|| < \delta$ fulfill $||x(t) - x^0(t)|| < \epsilon$ for all $t \geq t_0$ where $||.||$ is a suitable *vector norm.*

Asymptotic stability, weak sense:

The solution $x^0(t)$ of Eq.(37) is asymptotically stable if it is stable and $||x(t) - x^0(t)|| \to 0$ when $t \to \infty$ provided that $||x(t_0) - x^0(t_0)||$ is small enough.

Note that stability is a *property of a solution* for nonlinear systems.

In the case of input-affin nonlinear systems we assume that $f(x,t) = f(x)$ and $f(0) = 0$. Then Eq.(37) has a stationary solution $x^0(t) \equiv 0$ for $x^0(t_0) = 0$. In this case the notion of *asymptotic stability* is used in a more strict sense.

Asymptotic stability, strong sense:

Eq.(37) is asymptotically stable if $||x(t)|| \to 0$ when $t \to \infty$ provided that $||x(t_0)||$ is small enough.

Since our mathematical model is in the input-affin form, asymptotic stability in strong sense is investigated.

As we mentioned earlier there are some techniques which are easy to apply to input-affin models. Let's get acquainted with two of them. The *contraction technique* checks the contractive property of the state function f with the help of its Jacobian. The Lyapunov technique uses a generalized energy function computed from the state variables. Our goal is then to find an appropriate Lyapunov function which satisfies some requirements.

4.1.1 Contraction technique [5]

A notion for proving stability is the property called *contractiveness*. Let us given the truncated nonlinear state equation in the form of

$$\frac{dx}{dt} = f(x,t) \tag{38}$$

A region of state space is called a contraction region if the Jacobian of f is uniformly negative definite on it. In this case, function f is called a contraction in this region.
A system in input-affin form with contractive state function f is asymptotically stable.

Contractiveness can be proved by the negative definiteness of the Jacobian of state function f with computing the eigenvalues. If all of them have negative real parts, then contractiveness and therefore stability is proved. Allowing eigenvalues with zero real parts semi-contractiveness of f and consequently a system on the boundary of stability is found.

4.1.2 Lyapunov technique [2]

In stable conservative systems "energy" is a positive definite scalar function which should decrease with time. This aspect gives rise to a generalized energy or *Lyapunov* function $V[x]$ with the following properties:

1. *scalar function*

$$V \ : \ \mathbf{R}^n \ \rightarrow \ \mathbf{R}^+$$

2. *positive definite*

$$V[x(t)] > 0$$

3. *dissipative*

$$\frac{d}{dt}V[x(t)] = \frac{\partial V}{\partial x}\frac{d[x(t)]}{dt} < 0$$

If there exists a Lyapunov function for a system with the properties above, then the system is asymptotically stable.

Note that Lyapunov technique uses *centralized* variables that is $\overline{x}_i = x_i - x_{i_0}$ where x_{i_0} is the steady state of variable x_i.

4.2 Stability analysis of the evaporator system

In this section we have arrived to the stability investigation of the evaporator system model. We have some guesses about it: The system must be stable because all the energy and mass is taken to and from the vessel is associated with the input variables, which are set to zero during stability analysis. In consequence, the small disturbances are moving the system to another states and -because the system is closed-, it cannot get back to the original state. That means the system is on the boundary of stability.

First, let us get acquainted with a simplified model of the evaporator system! This is a DAE model consisting of four differential and three algebraic equations. The simplification is on the physico-chemical properties which are considered as constants. This is a model with differential index 1, moreover the constitutive equations can be substituted into the differential ones. The model equations obtained by *elimimating* the algebraic part are in the following form:

$$\frac{M_L}{dt} = -kA\ (\ P_0 exp(-\frac{C_1 cp_L M_L}{U_L}) - \frac{\rho_L R}{m_\omega cp_V}\frac{U_V}{V_T\rho_L - M_L}\ ) + \mathbf{F} - \mathbf{L} \tag{39}$$

$$\frac{M_V}{dt} = kA\ (\ P_0 exp(-\frac{C_1 cp_L M_L}{U_L}) - \frac{\rho_L R}{m_\omega cpV}\frac{U_V}{V_T\rho_L - M_L}\ ) - \mathbf{V} \tag{40}$$

$$\begin{aligned}\frac{dU_L}{dt} = &-kA\ (\ P_0 exp(-\frac{C_1 cp_L M_L}{U_L}) - \frac{\rho_L R}{m_\omega cp_V}\frac{U_V}{V_T\rho_L - M_L}\ )h_{LV} \\ &+uA\ (\ \frac{U_L}{M_L cp_L} - \frac{U_V}{M_V cp_V}\ ) + h_F\mathbf{F} - h_L\mathbf{L} + \mathbf{Q}\end{aligned} \tag{41}$$

$$\frac{dU_V}{dt} = kA\ (\ P_0 exp(-\frac{C_1 cp_L M_L}{U_L}) - \frac{\rho_L R}{m_\omega cpV}\frac{U_V}{V_T\rho_L - M_L}\ )h_{LV} + uA\ (\ \frac{U_L}{M_L cp_L} - \frac{U_V}{M_V cp_V}\ ) - h_V\mathbf{V} \tag{42}$$

In the other hand, another state space model can also be derived by *differentiating* the algebraic equations with respect to time:

$$\frac{dM_L}{dt} = -kA\ (\ P_0 exp(-\frac{C_1}{T_L}) - P\ ) + \mathbf{F} - \mathbf{L} \tag{43}$$

$$\frac{dM_V}{dt} = kA\ (\ P_0 exp(-\frac{C_1}{T_L}) - P\ ) - \mathbf{V} \tag{44}$$

$$\frac{dU_L}{dt} = -kA\ (\ P_0 exp(-\frac{C_1}{T_L}) - P\ )h_{LV} + uA\ (\ Tl - Tv\ ) + h_F\mathbf{F} - h_L\mathbf{L} + \mathbf{Q} \tag{45}$$

$$\frac{dU_V}{dt} = kA\ (\ P_0 exp(-\frac{C_1}{T_L}) - P\ )h_{LV} + uA\ (\ T_L - T_V\ ) - h_V\mathbf{V} \tag{46}$$

$$\frac{dP}{dt} = \frac{\rho_L R}{m_\omega cp_V}\ \frac{(kA\ (\ P_0 exp(-\frac{C_1}{T_L}) - P\ )h_{LV} + uA\ (\ T_L - T_V\ ) - h_V\mathbf{V})(V_T\rho_L - M_L)}{(V_T\rho_L - M_L)^2} + + \frac{(-kA\ (\ P_0 exp(-\frac{C_1}{T_L}) - P\ ) + \mathbf{F} - \mathbf{L})U_V}{(V_T\rho_L - M_L)^2} \tag{47}$$

$$\frac{dT_L}{dt} = \frac{cp_L\ (kA(exp(-\frac{C1}{T_L}) - P)(U_L - h_{LV}M_L) - uA(T_L - T_V)M_L}{(M_L cp_L)^2} + + \frac{M_L(h_F\mathbf{F} - h_L\mathbf{L} + \mathbf{Q}) - U_L(\mathbf{F} - \mathbf{L})\ )}{(M_L cp_L)^2} \tag{48}$$

$$\frac{dT_V}{dt} = \frac{cp_V\ (kA(exp(-\frac{C1}{T_L}) - P)(h_{LV}M_V - U_V) + uA(T_L - T_V)M_V}{(M_V cp_V)^2} + + \frac{\mathbf{V}(U_V - h_V M_V)\ )}{(M_V cp_V)^2} \tag{49}$$

4.2.1 Application of contraction technique

Let us investigate the asymptotic stability of these two state space models by contraction technique! Are the eigenvalues of the Jacobian of an operating point similar in these two models? First, let us consider how it works in the linear case!

Comparison of the two different state space representations in linear case

We are given a linear DAE model representation in the following form:

$$\begin{array}{rcl} \frac{dx}{dt} & = & A_{11}x \ + \ A_{12}z \ + B_1u \\ 0 & = & A_{21}x \ + \ A_{22}z \end{array} \tag{50}$$

where $x \in \mathbf{R^n}$ is the vector of differential, $z \in \mathbf{R^m}$ is the vector of algebraic variables. For models with differential index 1 (in this case A_{22} is invertible), the algebraic equations can be substituted into the differential ones by expressing z from the second equation:

$$z = -A_{22}^{-1}A_{21}x \tag{51}$$

Using this, we get the state space model of dimension n in the following form:

$$\frac{dx}{dt} = (A_{11} - A_{12}A_{22}^{-1}A_{21})x + B_1u \tag{52}$$

The other way of deriving a state space representation is differentiating the algebraic part of the DAE representation with respect to time. Differentiating Eq.(51) we get an equation consistig of the time-derivative of z:

$$\frac{dz}{dt} = -A_{22}^{-1}A_{21}\frac{dx}{dt} = -A_{22}^{-1}A_{21}(A_{11}x + A_{12}z + B_1u) \tag{53}$$

From this, we can determine the state space representation of $n+m$ dimension given by differentiating the algebraic equations:

$$\frac{d}{dt}\begin{bmatrix} x \\ z \end{bmatrix} \ = \ \begin{bmatrix} A_{11} & A_{12} \\ -A_{22}^{-1}A_{21}A_{11} & -A_{22}^{-1}A_{21}A_{22} \end{bmatrix} \ \begin{bmatrix} x \\ z \end{bmatrix} \ + \ \begin{bmatrix} B_1 \\ 0 \end{bmatrix} u \tag{54}$$

If we take a look at this state equation, we can recognize that the second row of the state matrix is the linear combination of the first row:

$$[-A_{22}^{-1}A_{21}A_{11} \quad -A_{22}^{-1}A_{21}A_{12}] = -A_{22}^{-1}A_{21}[A_{11} \quad A_{12}] \tag{55}$$

From this fact, it comes that the latter model has (at least) m zero eigenvalues.

Note that we suspect that the state matrices of these two models represented by Eq.(52) and Eq.(54) have n identical eigenvalues, and the proof will be a subject of research in the future.

Application of contraction technique to the evaporator system model Let us investigate the stability of the evaporator system given by two different representations!

A Maple script called Munkapont.mws is written for investigating the eigenvalues in both cases. This script can be found in the Appendix as Munkapont.mws.

Applying contraction technique to different operating points of the system we found that the eiqenvalues of the state space model derived by differentiation are identical to the model derived by substitution, with appropriate number of additional zero eigenvalues. Table (7). shows this situation for different operating points. Column 'eigenvals1' contains the eigenvalues of the model derived by substitution, while 'eigenvals2' belongs to the model derived by differentiation. Table (7). contains three examples with operating point for inputs $\mathbf{F} = 1\ kg/s$, $\mathbf{L} = 0.9\ kg/s$ $\mathbf{V} = 0.1\ kg/s$, $\mathbf{Q} = 101.724\ kJ/s$. Note that during computation numerical errors occurred with the maximal size of 10^{-6}. (Compare with Table 10. in section 5.3.)

$M_L\ [kg]$	$U_L\ [kJ]$	$M_V\ [kg]$	$U_V\ [kJ]$	eigenvalues 1	eigenvalues 2
800	1142400	0.2023	95.366	-68.212,-4700.888,0,0	-68.212,-4700.888,0,0,0,0,0
800	1200000	0.4021	199.118	-68.02,-2502.414,0,0	-68.02,-2502.414,0,0,0,0,0
1000	1386000	0.1686	79.4718	-81.673,-5641.33,0,0	-81.673,-5641.33,0,0,0,0,0

Table 7: Eigenvalues of the two models for different operating points.

As the real parts of the eigenvalues are negative or zero, the system is on the boundary of stability. We have showed, that the system is *not* asymptotically stable, but fulfills the requirements of boundary input-boundary output (BIBO) stability.

4.2.2 Application of Lyapunov technique

If we went on nvestigating, the other way we would use for proving stability is the Lyapunov technique. In applying this technique, we usually search a Lyapunov function in the following quadratic form:

$$V[x(t)] := \overline{x}^T P \overline{x}$$

where P a positive definite symmetric matrix, and x is are the centralized state vector. The most simple case is when P is a positive definite diagonal matrix. In

this special case the form of the Lyapunov function is the following:

$$V[x(t)] = \frac{1}{2} \sum w_i \overline{x}_i^2,$$

where w_i -s are positive constants (weights), and x_i -s are the components the of the state vector. In this form the first and second properties (positive definite scalar function) are fulfilled automatically. The emphasis is on the third property: The time-derivative of V must be negative:

$$\frac{d}{dt} V[x(t)] = \sum \overline{x}_i \frac{d\overline{x}_i}{dt} < 0 \tag{56}$$

The third property (dissipativity) and therefore asymptotic stability can be checked for a concrete operating point using (56).

Since we know that our system is not asymptotically stable, we are surely not able to find an appropriate Lyapunov function to the system.

5 Simulations

Equipped with the theory in the previous chapters, this chapter shows practical results. The evaporator system is simulated in Matlab's SIMULINK toolbox to show the behaviour of state variables in different situations. First, this model is introduced and explained carefully.

As defined in the latest chapter, asymptotic stability is a property of an operating point. Therefore we wonder if the system has any steady state(s) or not. To answer this question, a Maple script is written. Using this script, an operating point is found and used for further investigation. Finally, we examine whether the state variables are convergent to this point on a small neighbourhood of this point.

5.1 The evaporator model used in simulations

In order to make the analysis easier, we make some simplifications on our system: the physico-chemical properties are considered as constants. This assumption gives rise to algebraic equations which are completely substitutable into the differentials. This way we get a purely differential four-equation model with four differential variables as M_L, M_V, U_L, U_V for this special case:

$$\frac{dM_L}{dt} = -kA(P^* - P) + \mathbf{F} - \mathbf{L} \tag{57}$$

$$\frac{dM_V}{dt} = kA(P^* - P) - \mathbf{V} \tag{58}$$

$$\frac{dU_L}{dt} = -kA(P^* - P)h_{LV} - uA(\frac{U_L}{M_L cp_L} - \frac{U_V}{M_V cp_V}) - \mathbf{L}h_L + \mathbf{F}h_F + \mathbf{Q} \tag{59}$$

$$\frac{dU_V}{dt} = kA(P^* - P)h_{LV} + uA(\frac{U_L}{M_L cp_L} - \frac{U_V}{M_V cp_V}) - \mathbf{V}h_V \tag{60}$$

where

$$P^* = P_0 exp(-C_1 \frac{M_L cp_L}{U_L}) \tag{61}$$

NAME	DESCRIPTION	VALUE	UNITS
k	mass transfer coefficient	0.55	$kg/(kPa \cdot s)$
u	energy transfer coefficient	1240.58	$kJ/(m^2 \cdot s \cdot K)$
c_{pl}	specific heat of liquid (water)	4.18	$kJ/(kg \cdot K)$
c_{pv}	specific heat of vapour	1.386	$kJ/(kg \cdot K)$
h_L	liquid specific enthalpy	1428	kJ/kg
h_V	vapour specific enthalpy	471.24	kJ/kg
h_F	feed specific enthalpy	1230.6	kJ/kg
h_{LV}	interphase vapour spec. enthalpy	2255.6	kJ/kg
A	interfacial area	1	m^2
V_T	the volume of the vessel	2	m^3
ρ_L	density of liquid (water)	1000	kg/m^3
P_0	coefficient	113378958.9	kPa
C_1	coefficient	5189.371	$1/K$
R	universal gas constant	0.008314	$kJ/(mol \cdot K)$
M_ω	molecular weight of water	0.018	kg/mol

Table 8: Table of Constants

and

$$P = \frac{\rho_L R}{m_\omega c p_V} \frac{U_V}{V_T \rho_L - M_L} \tag{62}$$

This model can be used much easier for the purpose of simulation, and the Simulink model being introduced soon is built up on it.
The masses and energies M_L, M_V and U_L, U_V are measured in [kg] and [kJ], F, L, V and Q are given in [kg/s] and [kJ/s], respectively. Table 8. contains all the numerical data used.

5.2 The SIMULINK model of the evaporator

As seen in Figure 2., the Simulink representation of our mathematical model consists of long wires and different "boxes". The former ones represent variables - for example M_V and $\dot{M}_V$ are denoted by `Mv and dMv` -, the latter ones represent functional units

as integrators, functions, inputs, displays etc.

There are two main batches of wires in the model. The right one contains the input variables as it seen at the top of the model (boxes named "F","L","V","Q"). The left batch contains the state variables as Uv, Ul, Mv, Ml from left to right. The computation of them happens in four closed-loop units. The first one computes the variable M_L. If we take a look at this block, we can see that the two batches join to a multiplexer which outputs an eight-valued vector. It goes into a "function" block called `dMl`, where the computation of $\dot{M}_L$ is performed. The edge that connects it with an integrator carries the actual value of `dMl`. From the integrator, we get back the computed value of M_L which is carried and looped back to its wire in the batch. The actual value of state variables is stored in every step and taken into vectors with the help of "To Workspace" blocks.

We can set the values of input variables in the boxes at the top. Before running a simulation we can set the initial values of state variables at the integrator blocks.

5.3 Steady-state operating points of the evaporator

In order to be able to investigate asymptotic stability, we have to search for a steady-state operating point. This section concerns with this question.

The computation of an operating point seems very simple using that the derivatives are zero in steady state. Thus, we can consider our differential equations (57)-(60) as algebraic equations with specified variables $\dot{M}_L, \dot{M}_V, \dot{U}_L, \dot{U}_V$ set to zero:

$$-kA(P^* - P) + \mathbf{F} - \mathbf{L} = 0 \tag{63}$$

$$kA(P^* - P) - \mathbf{V} = 0 \tag{64}$$

$$-kA(P^* - P)h_{LV} - uA(\frac{U_L}{M_L cp_L} - \frac{U_V}{M_V cp_V}) - \mathbf{L}h_L + \mathbf{F}h_F + \mathbf{Q} = 0 \tag{65}$$

$$kA(P^* - P)h_{LV} + uA(\frac{U_L}{M_L cp_L} - \frac{U_V}{M_V cp_V}) - \mathbf{V}h_V = 0 \tag{66}$$

If we take a look at these equations we can find that the structural rank of this equation set reduces to 2 from the general case 4 (the case before specification). It means there are over-and under-determined parts in the set of variables. Table 9. depicts this situation.

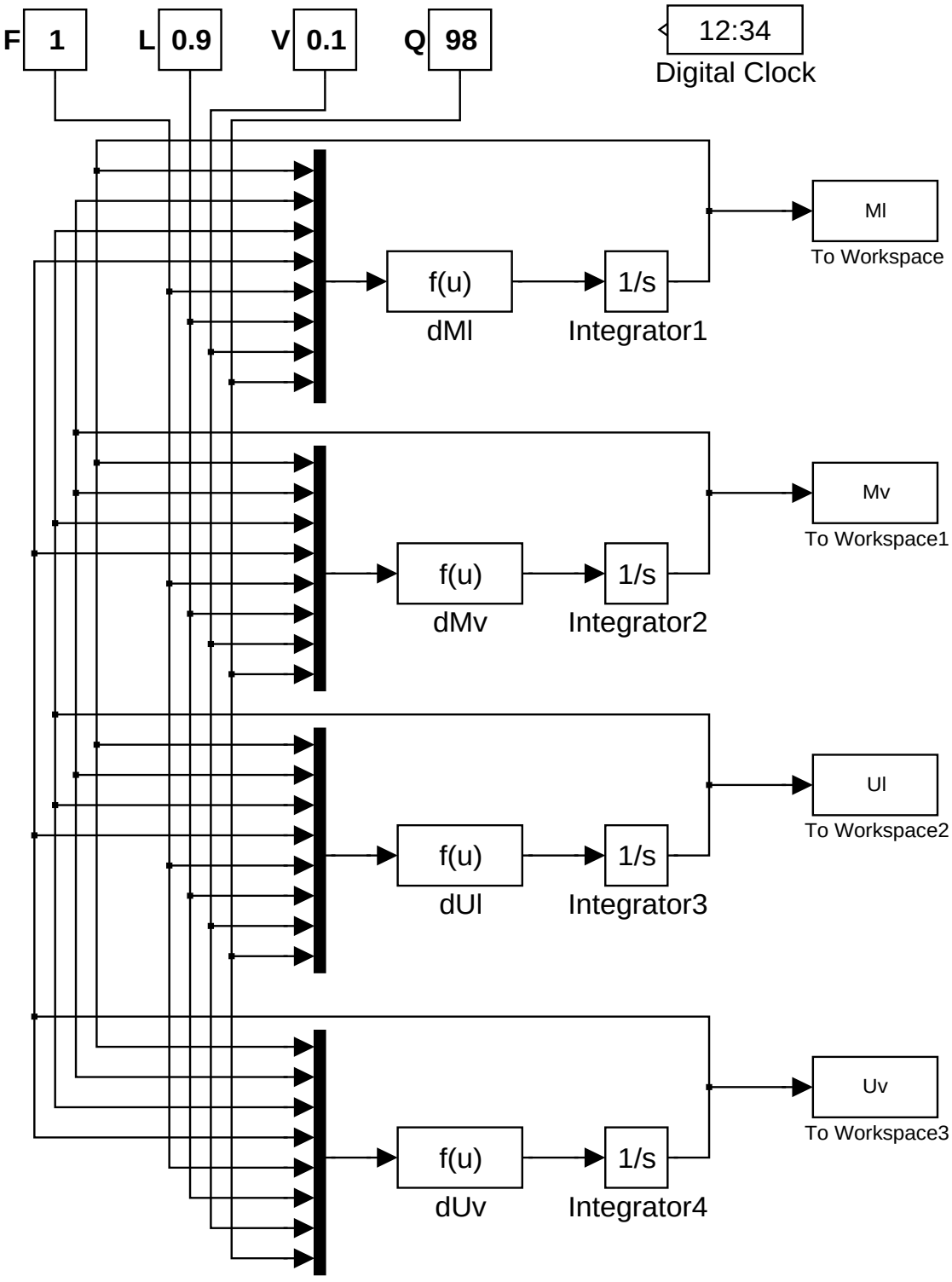

Figure 2: The Simulink model of the evaporator system

	M_L	M_V	U_L	U_V	$\dot{M}_L$	$\dot{M}_V$	$\dot{U}_L$	$\dot{U}_V$	**F**	**L**	**V**	**Q**
57	X		X	X	0				X	X		
58	X		X	X		0					X	
59	X	X	X	X			0		X	X		X
60	X	X	X	X				0			X	

Table 9: Singular algebraic equation set for computing operating points

The problem is easy to see: If we specify the variables $\dot{M}_L, \dot{M}_V, \dot{U}_L, \dot{U}_V$ as zeroes (denoted by 0's in the structure matrix), both the equation set containing Eq.(57)-(58) and the set containing Eq.(59)-(60) become singular.

The under-determined parts of equations contain the variables M_L, M_V, U_L, U_V. These parts of equations are linearly dependent in both of the equations sets. The over-determined parts of equations are related to the input variables $\mathbf{F}, \mathbf{L}, \mathbf{V}, \mathbf{Q}$.

The latter problem is easy to handle: we can choose only two input variables, if we want to get to a steady state. The relationship is given by the following equations:

$$\mathbf{F} - \mathbf{L} - \mathbf{V} = 0 \tag{67}$$

$$-\mathbf{L}h_L + \mathbf{F}h_F + \mathbf{V}h_v + \mathbf{Q} = 0 \tag{68}$$

If we fulfill these relations we surely get to an operating point.

Our bigger problem is the former: the original equations are singular, with the rank of two. That means endless number of steady states depending on initial conditions. This problem can be managed by reducing the set of input variables and using a valve or a free outflow instead which are functions of state variables.

Now we insist on generality, therefore we go on another way: we give two input and two state values (e.g. $\mathbf{F}$, $\mathbf{L}$, M_L, U_L) in our specification, and compute the other part from the equations. In the Appendix, the Maple script called Munkapont.mws (mentioned earlier in Chapter 4.2.) is written to show how it works in practice. For this case, the values of variables are specified as:

$$M_L = 800\ kg,\ U_L = 1142400\ kJ,\ \mathbf{F} = 1\ kg/s,\ \mathbf{L} = 0.9\ kg/s$$

The other part of state and input variables are computed:

$$M_V = 0.2023\ kg,\ U_V = 95.3661\ kJ,\ \mathbf{V} = 0.1\ kg/s,\ \mathbf{Q} = 101.724\ kJ/s$$

Several operating points are shown in Table 10. The states and inputs determined by us are situated on the left, the other (computed) part is on the right. In the Maple script the first example in Table 10. had been used.

M_L $[kg]$	U_L $[kJ]$	$\mathbf{F}$ $[kg/s]$	$\mathbf{L}$ $[kg/s]$	M_V $[kg]$	U_V $[kJ]$	$\mathbf{V}$ $[kg/s]$	$\mathbf{Q}$ $[kJ/s]$
800	1142400	1	0.9	0.2023	95.366	0.1	101.724
800	1200000	1	0.9	0.4021	199.118	0.1	101.724
1000	1386000	0.3	0.29	0.1100	50.332	0.01	49.652
1000	1386000	0.3	0.25	0.1095	50.1142	0.05	11.382
1000	1386000	0.3	0.3	0.1102	50.387	0	59.22

Table 10: Operating points for different values of specification

5.4 Simulation results

This time we have all the means for making simulations and investigating the results that we are given.

First, let's see a system which fulfills Eq.(67) and Eq.(68), so the existence of steady state is provided. We start simulation from two different initial states, and show that the steady states exist, but they are different.

Simulation 1. uses the input vector $[F, L, V, Q]^T = [1\frac{kg}{s},\ 0.9\frac{kg}{s},\ 0.1\frac{kg}{s},\ 101.7240\ \frac{kJ}{s}]$, which satisfies the conditions on inputs given by Eq.(67) and Eq.(68). Two cases are shown:

- Simulation 1.1 is started from the state $x_{0_1} = [M_{L_0}, M_{V_0}, U_{L_0}, U_{V_0}]^T = [1000\ kg, 1\ kg, 1400000\ kJ, 470\ kJ]^T$. The trajectories of state variables are depicted in Figure 3. The given steady state is

$$\overline{x_1} = [1000.875\ kg, 0.1252\ kg, 1400412.16\ kJ, 0.57841\ kJ]^T.$$

- Simulation 1.2 begins at $x_{0_2} = [600\ kg, 0.15\ kg, 1000000\ kJ, 65\ kJ]^T$. As shown in Figure 4., the simulation results in

$$\overline{x_2} = [598.297\ kg, 1.8532\ kg, 999043\ kJ, 1021.937\ kJ]^T.$$

As we can see starting from two different initial conditions we get different results: the steady state is not unique. It is because the equation set for computing the operating point is under-determined and therefore there are infinite different steady states: for different initial conditions we get different results. There is an infinite number of solutions depending on initial conditions.

If the conditions on input variables Eq.(67) and/or Eq.(68) are not satisfied (inputs are arbitrarily given), simulations lead to not converging trajectories.

Simulation 2. shows the trajectories obtained from a system which does not fulfill Eq.(68). As Figure 5. depicts, there is no steady state found in that case, so the system is unstable.

As we mentioned, the set of equations for determining the operating point of the system is under-determined: its degree of freedom is two instead of zero. If the values of two state variables are given by us, the degree of freedom equals to zero, and the other part of the operating point is unique!

Simulation 3. shows the example which for the Maple script is written. In this case, two components of the operating point is given: $M_L = 800\ kg$ and $U_L = 1142400\ kJ$. Try to find the steady state from different U_{L_0}, U_{V_0} initial conditions! As Figure 6. shows, the result of simulation is the same for three different initial states; the operating point is uniquely determined and independent of the initial conditions: $[\overline{M_V}, \overline{U_V}]^T = [0.2022\ kg, 95.366\ kJ]^T$.

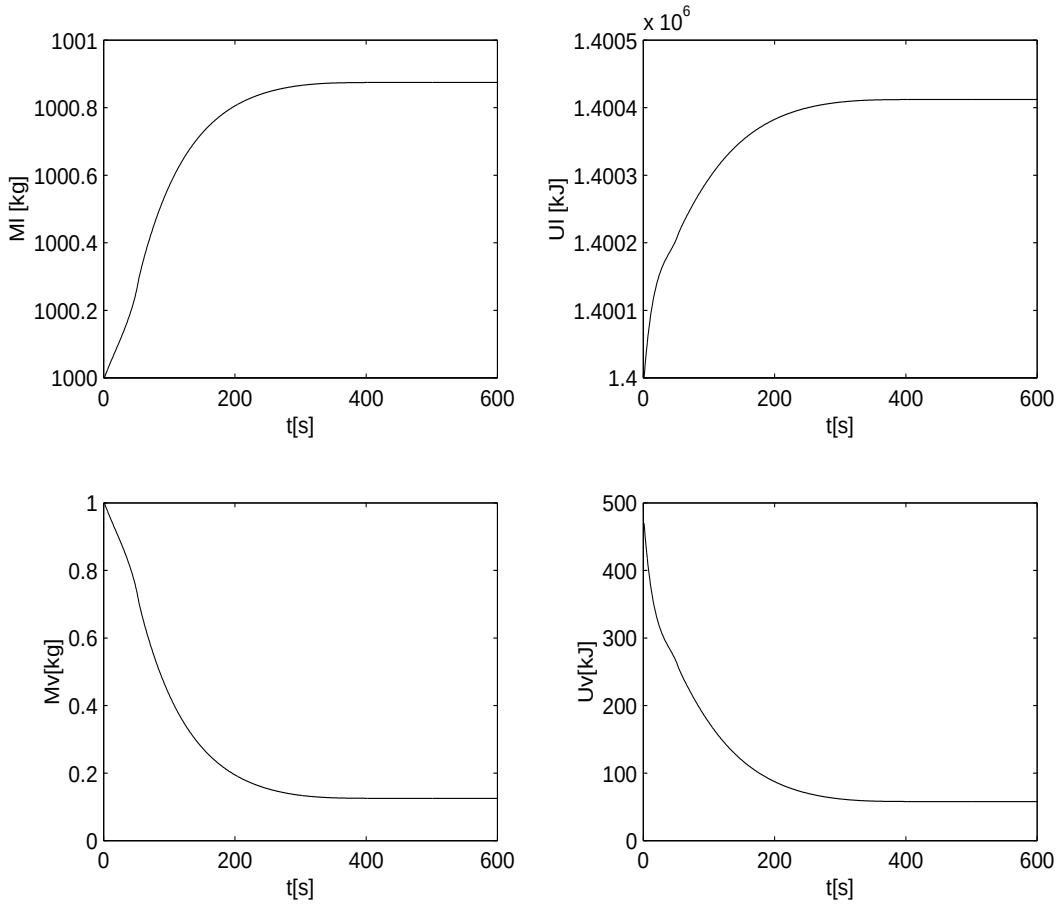

Figure 3: Simulation 1.1. Different initial conditions

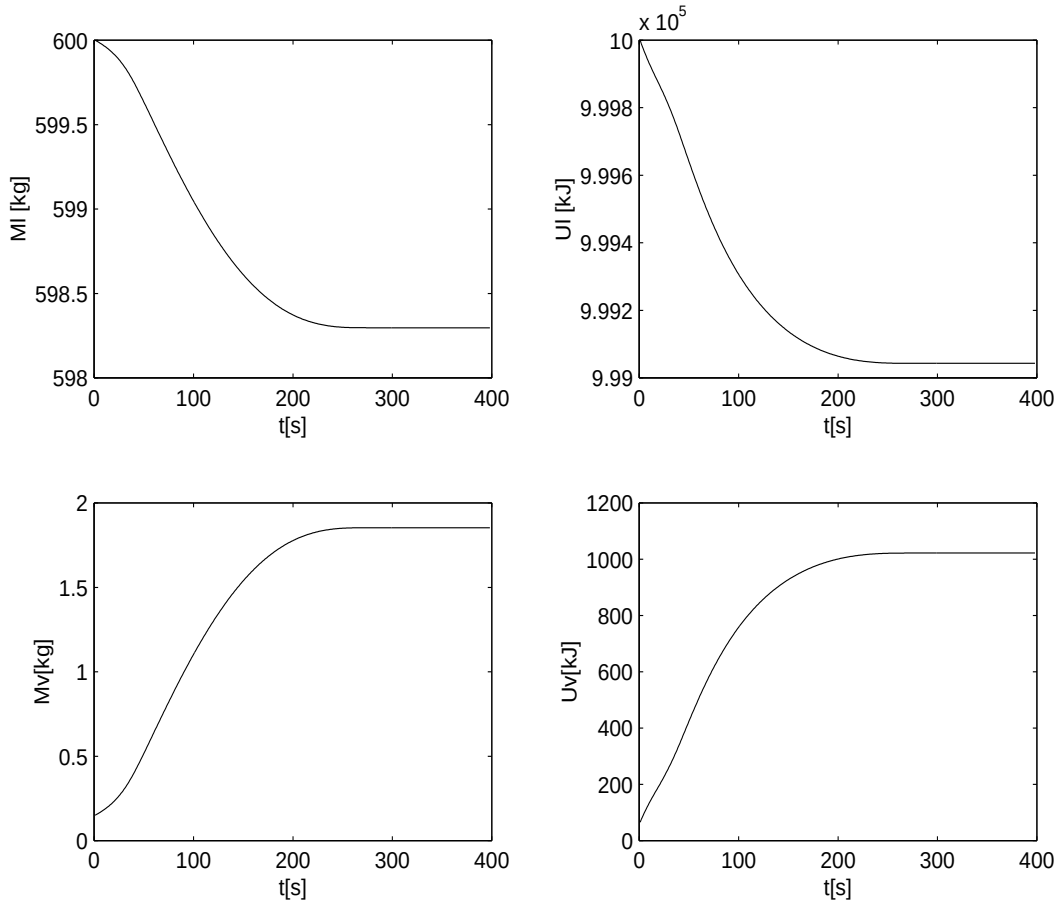

Figure 4: Simulation 1.2. Different initial conditions

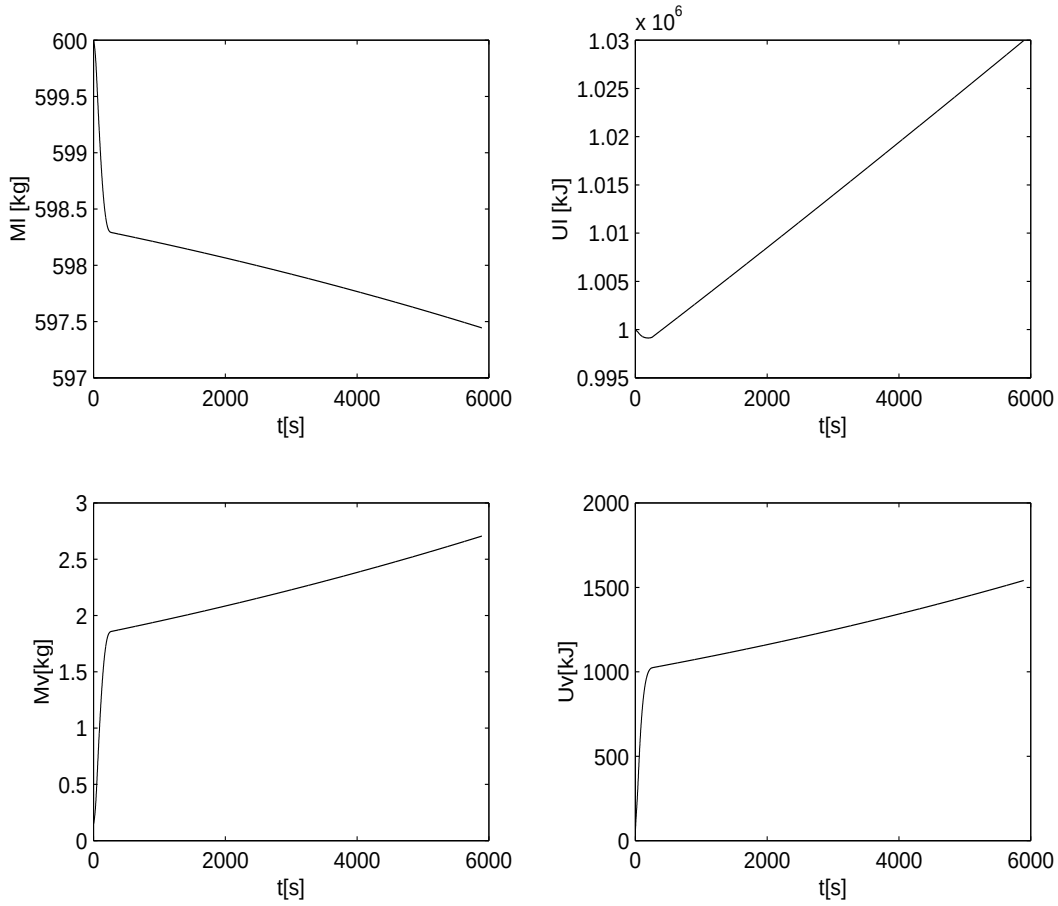

Figure 5: Simulation 2. Lack of steady state

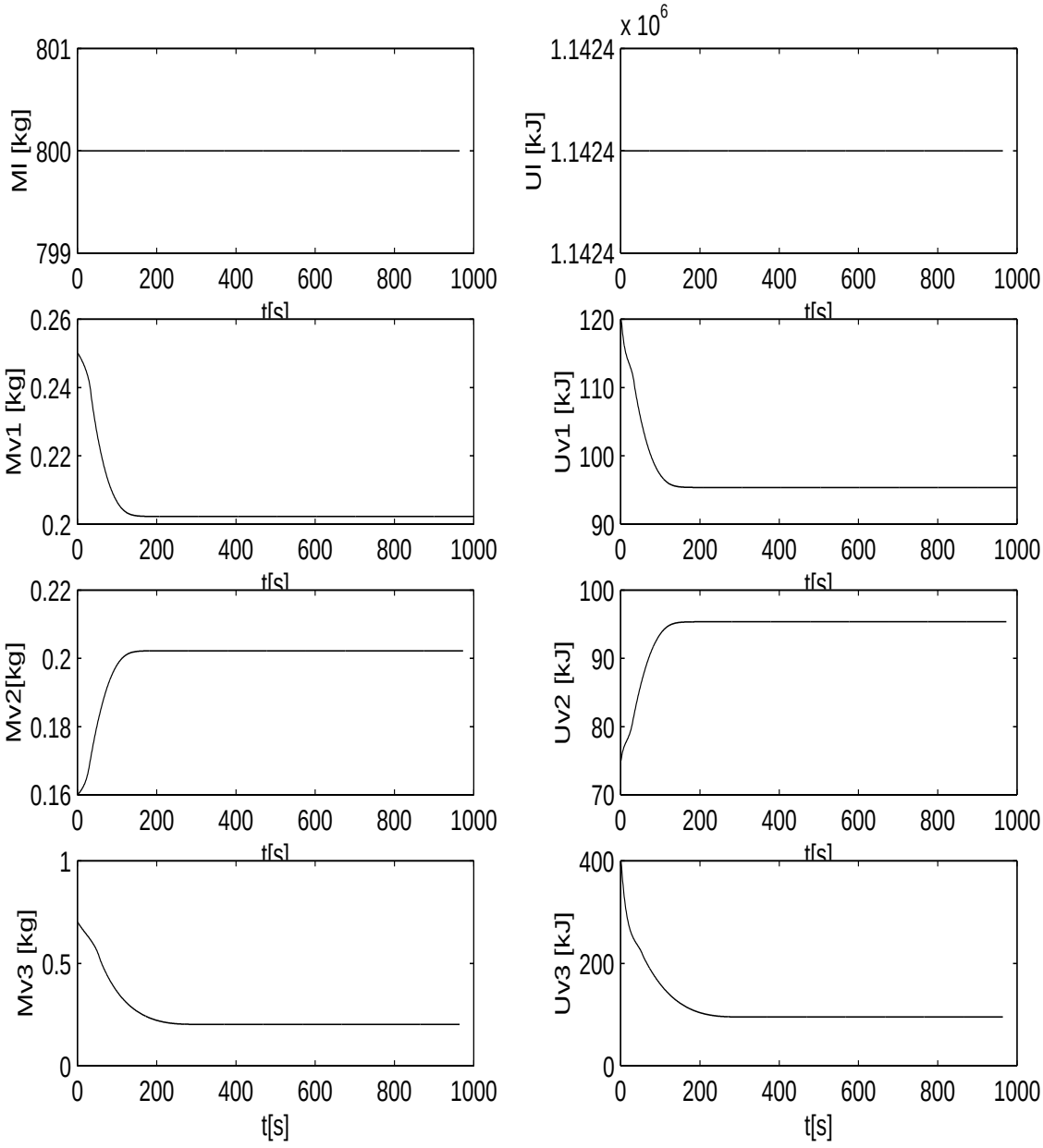

Figure 6: Simulation 3. Unique operating point

6 Conclusion and future work

We have achieved partial results in investigating asymptotic stability of process systems, where we examine the change of extensive (mass and internal energy of phases) and intensive (temperature) quantities around an operating point caused by the effect of external disturbances. Our approach is based on the basic principles of process systems, namely that process systems can be described by the laws of thermodynamics.

A typical example for a simple but hard-to-investigate class of process systems, a lumped parameter evaporator system of two phases with one physical input (liquid) and two physical outputs (vapour, liquid) has been chosen for the analysis. The dynamic model of the system is in the form of a differential-algebraic set of equations where the algebraic constitutive equations cannot be substituted into the differential ones.

The steps of our approach are the following.

1. *Construction of DAE process model of the system from first engineering principles*

   First we presented a mathematical investigation of asymptotic stability using the state space model of process systems. After constructing model equations we obtained a model in differential-algebraic equation (DAE) form consisting of differential equations and a sufficient number of algebraic equations. These relations are not always given in explicit form but computed by subroutines of special program packages.

   Since our tools can be applied to a model form of purely differential equations, especially to *input-affin* form, we set the target of eliminating all the constitutive algebraic equations with substituting them into the differential ones.

2. *Structural analysis of the algebraic part*

   On the second step with the help of structure matrices it was shown that the algebraic variables cannot be expressed from the algebraic equations and substituted into differential ones because of the multiple relations and the nonlinearity.

3. *Transformation of the DAE model into its state space equation form*
   By transforming five algebraic variables of the DAE model into the differential ones the variables remained became substitutable into the differential equations.

As a result, this method is applicable in all other cases where the same problem turns out. Thus, if a part of algebraic variables shown by blocks in the structure matrix is non-expressible, we can transform the coupled algebraic equations into differential ones by differentiation. The disadvantage of this method is getting a larger set of differential equations, which gives a chance of investigation, but unfortunately makes it more complex.

By then, we derived a dynamical set of equations for the evaporator system consisting of nine equations. In other system classes, e.g. mass convection networks, the state function of the mass balances doesn't depend on the other conservative variables which gives a possibility of decomposition. This way we can analyze two smaller subsystems instead of the big one. Our expectation was a model with the property above, but the decomposition was not successful. The causing factor was the energy transfer, so we came to the consequence that lack of decomposition is caused by transfer effect.

Decomposition can hopefully be done after an appropriate similarity transformation and that is a matter of research later on.

We wanted to determine the steady states of the system by considering the derivatives as zeroes. This method concluded in a set of equations, which is structurally solvable except the operating point. This led to over-and under-determined sets of variables. It has been shown that there is no unique operating point of the investigated mathematical model using the original natural set of input variables in the specification.

With the help of a Maple script, we have investigated the asymptotic stability of an operating point on the simplified index 1 model of the evaporator system by means of contraction technique. It was shown that the model received by substituting the algebraic equations into the differential ones, and the model obtained from differentiating the algebraic equations with respect to time have the same eigenvalues - completed with appropriate number of zero eigenvalues. It was shown that the system is on the boundary of stability.

As an additional result, for linear case we proved the completion of the eigenvalues of the state matrix A with zero eigenvalues of the number of algebraic equations.

The Lyapunov technique has also been used for checking asymptotic stability by searching for an appropriate Lyapunov function of the system. In our case we obtained an inequality of first degree with unspecified nonlinear functions therefore no definite answer has been found on the stability question. We are in principle satisfied with this final result which can be applied to other concrete similar examples.

In the future there are several topics to be investigated:

1. We did not give up the idea of decomposition and do want to realize that by finding a similarity transformation which transforms the system to a decomposable one.

2. As we want to know more on restrictions for stability characterized by the inequality, we go on analyzing that from different points of view later on.

3. For the linear case, we investigated a general linear model in DAE form. We derived state space models by two methods: with eliminating, and differentiating the algebraic equations. The identicalness of eigenvalues of the state matrices of these two different representations is not proved yet. We want to complete the proof, and generalize this theorem for nonlinear DAE models.

4. Asymptotic stability is an important quality of a process system, but we have not said anything about the non-determined potential input variables F, V, L and Q yet. These quantities were considered as disturbances, but we can consider them as input variables. Inventing different controllers to get relationship between the input and the state variables into the state equations, the system trajectories can be analyzed.

5. As a concrete application with great importance, we want to find a new way to construct stabilizing controllers for the system.

6. Only a simple example of a process model class has been investigated in this report. Of course our purpose is wider - we want to generalize the given results and induce them to other classes of models.

References

[1] K. M. Hangos and I. T. Cameron. *Process Modelling and Model Analysis*. Academic Press, 2001.

[2] Katalin Hangos, József Bokor, and Miklós Gerzson. *Computer Controlled Systems*. Veszprémi Egyetemi Kiadó, Veszprém, 1995.

[3] Katalin Hangos, József Bokor, and Gábor Szederkényi. Analysis and control of nonlinear process systems. Technical report, SCL-1/99 *Computer and Automation Research Institute, Hungarian Academy of Sciences*, 1999.

[4] A. Kumar and P. Daoutidis. *Control of nonlinear differential algebraic equation systems*. Chapman and Hall/CRC, London, 1999.

[5] W. Lohmiller and J. E. Slotine. Nonlinear process control using contraction theory. *AIChE Journal*, 46:588–596, 2000.

[6] Herbert Sira-Ramirez. A general canonical form for feedback passivity of nonlinear systems. *International Journal of Chemistry*, 71:891–905, 1998.

[7] Zs. Tuza, G. Szederkényi, and K.M. Hangos. The effect of modeling assumptions on the differential index of lumped process models. Technical report, *Computer and Automation Research Institute, Hungarian Academy of Sciences, 2000.*

Appendix