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For questions during the exam:
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Exam in TTK4130 Modeling and Simulation

Monday, May 15 2017
09:00 – 13:00

Permitted aids (code A): All written and handwritten examination support materials are permitted.

Answers in English, Norwegian, or a mixture of the two accepted.

Grades available: As specified by regulations.

Problem 1 (19 %)

Consider the following variable-step Runge-Kutta method with the extended Butcher tableau:

$$\begin{array}{c|cc} 0 & & \\ 2/3 & 2/3 & \\ \hline & 1/4 & 3/4 \\ & 1 & 0 \end{array}.$$

The following Taylor's expansion may be of use:

$$\mathbf{f}(\mathbf{y}_n + h\alpha\mathbf{k}, t_n + \alpha h) = \mathbf{f}(\mathbf{y}_n, t_n) + \alpha h \frac{d\mathbf{f}}{dt}(\mathbf{y}_n, t_n) + O(h^2). \tag{1}$$

(2 %) (a) Is the method explicit or implicit? Explain!

> **Solution:** It is an explicit method, since the Butcher array does not have values on or above the diagonal.

(2 %) (b) Find the order of the Runge-Kutta method with fewer stages (explanation required).

> **Solution:** The lower order method is the explicit Euler method. The Taylor-Series expansion is
> $$\mathbf{y}_{n+1} = \mathbf{y}_n + h\mathbf{f}(\mathbf{y}_n, t_n), \tag{2}$$
> which shows it is of order $p = 1$.

(5 %) (c) Find the order of the other Runge-Kutta method (calculations required).

> **Solution:** For the higher order method from the Butcher tableau it can be taken:
> $$\mathbf{k}_1 = \mathbf{f}(\mathbf{y}_n, t_n), \tag{3a}$$
> $$\mathbf{k}_2 = \mathbf{f}(\mathbf{y}_n + \frac{2}{3}h\mathbf{k}_1, t_n + \frac{2}{3}h), \tag{3b}$$
> $$\mathbf{y}_{n+1} = \mathbf{y}_n + h\left(\frac{1}{4}\mathbf{k}_1 + \frac{3}{4}\mathbf{k}_2\right). \tag{3c}$$

With the given Taylor's series expansion $\mathbf{k}_2$ can be calculated

$$\mathbf{k}_2 = f(\mathbf{y}_n, t_n) + \frac{2}{3}h\frac{d\mathbf{f}}{dt}(\mathbf{y}_n, t_n) + O(h^2). \tag{4}$$

With this the solution of the method is

$$\begin{aligned} \mathbf{y}_{n+1} =& \mathbf{y}_n + h\left(\frac{1}{4}\mathbf{f}(\mathbf{y}_n, t_n) + \frac{3}{4}\left[f(\mathbf{y}_n, t_n) + \frac{2}{3}h\frac{d\mathbf{f}}{dt}(\mathbf{y}_n, t_n) + O(h^2)\right]\right), && \text{(5a)} \\ =& \mathbf{y}_n + h\mathbf{f}(\mathbf{y}_n, t_n) + \frac{1}{2}h^2\frac{d\mathbf{f}}{dt}(\mathbf{y}_n, t_n) + O(h^3), && \text{(5b)} \end{aligned}$$

which shows the method is of order $p = 2$.

The following pendulum equation is given

$$\ddot{\theta} = -\frac{g}{l}\theta. \tag{6}$$

(6 %) (d) For which steplength h is the higher order method stable for the pendulum with length $l = 1m$ and $g = 10m/s^2$?

Solution: First the pendulum equation has to be transferred into state-space form. We use $x_1 = \theta$ and $x_2 = \dot{\theta}$. The state-space form is given by

$$\begin{pmatrix} \dot{x}_1 \\ \dot{x}_2 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -g/l & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}. \tag{7}$$

The eigenvalues of the system are $\lambda_{1/2} = \pm\sqrt{g/l}j$. (The Euler method is unstable for imaginary Eigenvalues). The higher order method has the stability function: $R(h\lambda) = 1 + \lambda h + \frac{1}{2}\lambda^2 h^2$ which can be seen from the previous part. Another option is to calculate it here with the stability function for explicit methods: $R(h\lambda) = det\left[\mathbf{I} - \lambda h\left(\mathbf{A} - \mathbf{1}\mathbf{b}^T\right)\right]$.
The stability function for the eigenvalues (only check $\lambda = +\sqrt{g/l}j$, as $-\sqrt{g/l}j$ will be the same) evaluates:

$$\begin{aligned} R\left(h\sqrt{g/l}\right) &= 1 + \sqrt{g/l}hj - \frac{1}{2}\frac{g}{l}h^2, && \text{(8a)} \\ &= \left(1 - \frac{1}{2}\frac{g}{l}h^2\right) + \sqrt{g/l}hj, && \text{(8b)} \end{aligned}$$

from which we see that

$$\begin{aligned} \left|R\left(h\sqrt{g/l}\right)\right| &= \sqrt{\left(1 - \frac{1}{2}\frac{g}{l}h^2\right)^2 + \left(\sqrt{g/l}h\right)^2}, && \text{(9a)} \\ &= \sqrt{1 + \frac{1}{4}\frac{g^2}{l^2}h^4} \overset{!}{\leq} 1. && \text{(9b)} \end{aligned}$$

The condition does not hold for any steplength. The method is always unstable for the pendulum.

(4 %) (e) This is the Butcher tableau of an *adaptive* method. Explain in a few sentences how the adaptivity of the method works and what advantages this includes.

Solution: The adaptive Runge-Kutta method approximates the local error vector $\mathbf{e}_{n+1}$ to adjust the steplength of the method. With this error estimate and a norm (for example the maximum norm) the local error $\varepsilon_{n+1} = \max_i |\mathbf{e}_{i,n+1}| = O(h^{p+1})$ can be found. This local error is compared to a user-defined tolerance e_{tol}. If $\varepsilon \gg e_{tol}$ the steplength is reduced, if $\varepsilon \ll e_{tol}$ the steplength is increased and if $\varepsilon \approx e_{tol}$ the steplength is retained.
The advantages are obvious: The user does not have to analyze the model/integration method to find an appropriate steplength. In non-adaptive methods the user would always have to choose the smallest steplength necessary, which (especially for nonlinear system) decreases the computations time in areas where a larger steplength would be sufficient for the required tolerance.

Problem 2 (14 %)

A pendulum (Fig. 1) was modeled with the Newton-Euler approach in the inertia system.

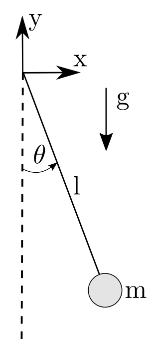


Figure 1: Pendulum.

The following DAE-system was derived

$$m\ddot{x} = -\frac{S}{l}x, \tag{10a}$$

$$m\ddot{y} = -\frac{S}{l}y - mg, \tag{10b}$$

$$0 = l^2 - x^2 - y^2, \tag{10c}$$

where S is the force in the rope.

(2 %) (a) Determine differential and algebraic variables of the system.

Solution: The differential variables are x, $\dot{x}$, y and $\dot{y}$. The algebraic variable is S.

(6 %) (b) Determine the differential index of the system.

Solution: We need to differentiate the algebraic equation to find a differential equation for the algebraic variable, since $\frac{\partial g(S)}{\partial S}$ is singular, which indicates the system is not index 1.
The first derivative of the algebraic equation becomes

$$0 = -2x\dot{x} - 2y\dot{y}, \tag{11a}$$

$$= -x\dot{x} - y\dot{y}. \tag{11b}$$

The second derivative of becomes

$$0 = -\dot{x}^2 - x\ddot{x} - \dot{y}^2 - y\ddot{y}, \tag{12}$$

where we can use the system equations (10). With this we get

$$0 = -\dot{x}^2 + x^2 \frac{S}{ml} - \dot{y}^2 + y^2 \frac{S}{ml} + yg, \tag{13a}$$

$$S = ml \frac{\dot{x}^2 + \dot{y}^2 - yg}{x^2 + y^2}. \tag{13b}$$

With the third derivative we get an ODE-system. Consequently, the system is of index 3.

(6 %) (c) Write down the Modelica code for the index 1 system based the system (10) and your results in the previous task. The name of the model should be `Pendulum`.
If you were not able to determine the index you can use only the system (10) (5%).

Solution: *Full score also if instead of SI units the* ***Real*** *variable is used. Moreover the gravity can also be defined as a* ***Real*** *parameter or constant.*

```
model Pendulum
  import SI = Modelica.SIunits;
  import G = Modelica.Constants.g_n;

  SI.Position x( start = 1);
  SI.Position y( start = 0);
  SI.Velocity vx( start = 0);
  SI.Velocity vy( start = 0);
  SI.Force S( start = 0);

  parameter SI.Length l = 1;
  parameter SI.Mass m = 1;

equation
   der(vx) = -S/m * x/l;
   der(vy) = -S/m * y/l - G;
   der(x) = vx;
   der(y) = vy;
   0 = S - m*l*(vx^2+vy^2 - y*G)/(x^2+y^2);
end Pendulum;
```

Problem 3 (30 %)

A hollow cylinder (mass m_1, radius R, $\delta << R$) is pivoted on two mass-less bearings. In the hollow cylinder a plate (mass m_2, radius r) rolls without sliding. The moments of inertia are denoted by I_i. The movement happens in a 2D plane (Fig. 2).

(2 %) (a) Find a connection between $\dot{\psi}$, $\dot{\phi}$ and $\dot{\theta}$.
Hint: If you are not able to find a connection, continue the task with the following: $(R+r)\dot{\phi} + r\dot{\psi} - R\dot{\theta} = 0$

Solution: Since the plate is not sliding the connection between angular velocities can be found by

$$(R - r)\dot{\theta} = R\dot{\psi} - r\dot{\phi}. \tag{14}$$

(2 %) (b) Why are ψ and θ a good choice as generalized coordinates?

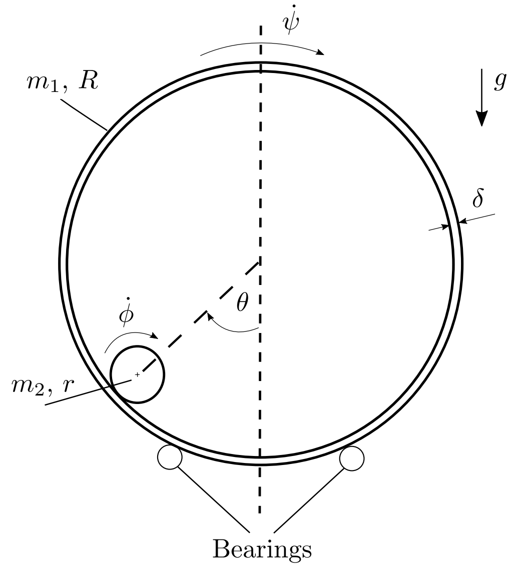


Figure 2: Hollow cylinder with rolling plate.

Solution: The system has two degrees of freedom. Therefore, two generalized coordinates are necessary to describe the system. The generate coordinates are:

$$q_1 = \psi, \quad q_2 = \theta. \tag{15}$$

(4 %) (c) Find the kinetic energy of the system.

Solution: The kinetic energy is given by

$$T = \frac{1}{2} I_1 \dot{\psi}^2 + \frac{1}{2} m_2 (R-r)^2 \dot{\theta}^2 + \frac{1}{2} I_2 \dot{\phi}^2. \tag{16}$$

With the connection between the angles found previously the kinetic energy is given as

$$T = \frac{1}{2} I_1 \dot{\psi}^2 + \frac{1}{2} m_2 (R-r)^2 \dot{\theta}^2 + \frac{1}{2} I_2 \left[\frac{R\dot{\psi} - (R-r)\dot{\theta}}{r} \right]^2 \tag{17}$$

(2 %) (d) Find the potential energy of the system.

Solution: The potential energy is given by

$$U = -m_2 g (R-r) \cos\theta \tag{18}$$

(8 %) (e) Find the equation of motion of the system.

Solution: The Lagrange equation of motion for this system

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i} - \frac{\partial L}{\partial q_i} = 0 \tag{19}$$

is used. L is defined as

$$L(\mathbf{q},\dot{\mathbf{q}},t) = T(\mathbf{q},\dot{\mathbf{q}},t) - U(\mathbf{q}), \tag{20}$$

where T is the kinetic energy and U the potential energy of the system. The Lagrangian is

$$L = \frac{1}{2}I_1\dot{\psi}^2 + \frac{1}{2}m_2(R-r)^2\dot{\theta}^2 + \frac{1}{2}I_2\left[\frac{R\dot{\psi}-(R-r)\dot{\theta}}{r}\right]^2 + m_2 g(R-r)\cos\theta \tag{21}$$

For $q_1 = \psi$:

$$\frac{\partial L}{\partial \psi} = 0, \tag{22a}$$

$$\frac{\partial L}{\partial \dot{\psi}} = I_1\dot{\psi} + I_2\frac{R}{r^2}\left[R\dot{\psi}-(R-r)\dot{\theta}\right], \tag{22b}$$

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\psi}}\right) = I_1\ddot{\psi} + I_2\frac{R}{r^2}\left[R\ddot{\psi}-(R-r)\ddot{\theta}\right], \tag{22c}$$

$$\ddot{\psi}\left[I_1 + I_2\left(\frac{R}{r}\right)^2\right] - I_2\frac{R(R-r)}{r^2}\ddot{\theta} = 0. \tag{22d}$$

For $q_2 = \theta$:

$$\frac{\partial L}{\partial \theta} = -m_2 g(R-r)\sin\theta, \tag{23a}$$

$$\frac{\partial L}{\partial \dot{\theta}} = m_2(R-r)^2\dot{\theta} - I_2\frac{R-r}{r^2}\left[R\dot{\psi}-(R-r)\dot{\theta}\right], \tag{23b}$$

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\theta}}\right) = m_2(R-r)^2\ddot{\theta} - I_2\frac{R-r}{r^2}\left[R\ddot{\psi}-(R-r)\ddot{\theta}\right], \tag{23c}$$

$$\ddot{\theta}(R-r)^2\left[m_2 + \frac{I_2}{r^2}\right] - I_2\frac{(R-r)R}{r^2}\ddot{\psi} + m_2 g(R-r)\sin\theta = 0. \tag{23d}$$

(6 %) (f) Determine the period of the oscillation in case of a small initial deflection in θ.

Solution: For a small deflection it holds: $\sin\theta \approx \theta$
The equation of motion becomes

$$\ddot{\theta}(R-r)^2\left[m_2 + \frac{I_2}{r^2}\right] - I_2\frac{(R-r)R}{r^2}\ddot{\psi} + m_2 g(R-r)\theta = 0. \tag{24}$$

For the equation of motion in (22d) we get

$$\ddot{\psi} = I_2\frac{R(R-r)}{I_1 r^2 + I_2 R^2}\ddot{\theta}. \tag{25}$$

Using (25) in (24) gives for small deflection the following equation of motion

$$\ddot{\theta} + \frac{m_2 g}{(R-r)\left(m_2 + \frac{I_2}{r^2} - \frac{R^2}{r^2}\frac{I_2^2}{I_1 r^2 + I_2 R^2}\right)}\theta = 0. \tag{26}$$

With (26) it follows

$$\omega^2 = \frac{m_2 g}{(R-r)\left(m_2 + \frac{I_2}{r^2} - \frac{R^2}{r^2}\frac{I_2^2}{I_1 r^2 + I_2 R^2}\right)}. \tag{27}$$

The period is given by $T = \frac{2\pi}{\omega}$:

$$T = 2\pi\sqrt{\frac{(R-r)\left(m_2 + \frac{I_2}{r^2} - \frac{R^2}{r^2}\frac{I_2^2}{I_1 r^2 + I_2 R^2}\right)}{m_2 g}} \tag{28}$$

(6 %) (g) Derive the moment of inertia for the hollow cylinder.
Hint: The derived moment of inertia should have a similar form as the moment of inertia of a rod: $I = \frac{1}{12}ml^2$ (*this task can be solved independently from the rest*).

Solution: The moment of inertia is given by

$$I = \int_Q r^2 dm, \tag{29}$$

where r is the distance from the rotation axis and Q the entire mass. The mass dm of a cylindrical body can be described by

$$dm = \rho dV = \rho L 2\pi r dr, \tag{30}$$

where L is the length and dr is the infinitesimal radius of the cylinder (Fig. 3).

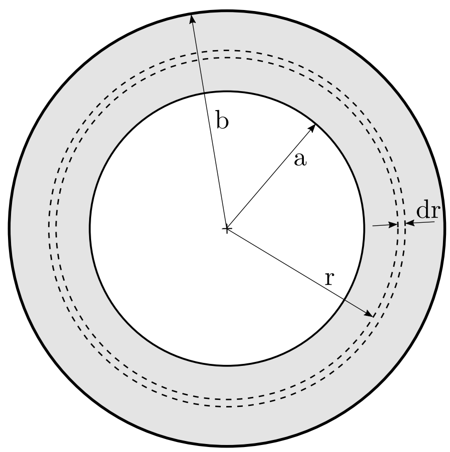


Figure 3: Infinitesimal radius of hollow cylinder.

The density of the hollow cylinder is

$$\rho = \frac{M}{L\pi(b^2 - a^2)}, \tag{31}$$

where M is the mass of the hollow cylinder.

The moment of inertia can be derived by solving the integral

$$I = 2\pi\rho L \int_a^b r^3 dr \tag{32a}$$

$$= 2\pi\rho L \left[\frac{b^4}{4} - \frac{a^4}{4}\right] \tag{32b}$$

$$= \frac{M}{2(b^2 - a^2)}[b^4 - a^4] \tag{32c}$$

$$= \frac{1}{2}M(b^2 + a^2), \tag{32d}$$

where it was used that $(b^4 - a^4) = (b^2 - a^2)(b^2 + a^2)$.
Since the cylinder is hollow $R = b \approx a$ which gives a moment of inertia for the hollow cylinder

$$I \approx MR^2 \tag{33}$$

Problem 4 (14 %)

A simulation model for an autonomous fire truck should be found. For test purposes a small scale model of the fire truck was build (Fig. 4).

Figure 4: Fire truck - Small scale model.

The project has several groups working on different parts of the model. Your task is to find the equation of motion of the ladder on the fire truck to precisely control the position of the hose outlet. The only subtask we will consider here is to find the connection between inertial coordinate frame, which is aligned with the truck, and the body frame of the hose.
The movement can be described by three rotation and one translation. Two rotations are in the attachment of the ladder to the truck. One of these rotations rotates the ladder around θ in the horizontal plane, the other rotates the ladder around ψ up or down. Afterward a translation $l(t)$ has to be performed from the attachment to the joint of the hose. The hose joint can be rotated around ϕ up or down.

(6 %) (a) In the first step the coordinate systems (inertial and body frames) have to be defined. Draw an abstraction (body diagram) of the process that shows the inertial coordinate system with the axes $(\{x_i, y_i, z_i\})$. The origin is in the attachment of the ladder and one axis is aligned with the vehicle. Furthermore, draw the two body coordinate systems with the axes $(\{x_a, y_a, z_a\})$ and $(\{x_b, y_b, z_b\})$.

The first body coordinate system is the one after the first rotation with its origin in the attachment. The second has its origin in the joint of the hose at the end of the ladder. Include in your drawing also the angular velocities $\dot{\theta}$, $\dot{\psi}$ and $\dot{\phi}$ and the translation $l(t)$.

Solution: One of the possible configuration is shown in Fig. 5. *Other configuration can also be correct. Important is to have a right-hand coordinate system and describe the rotation correctly in this frame.*

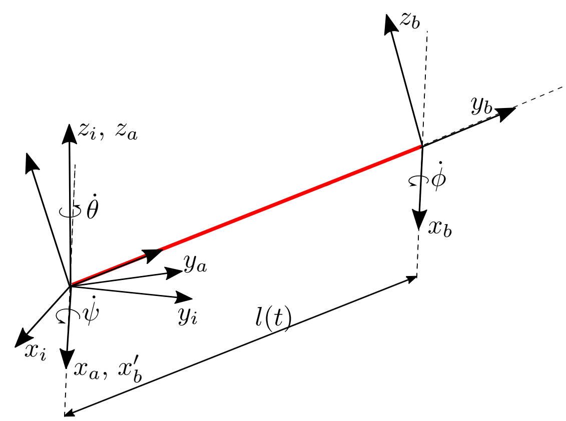


Figure 5: Abstraction of fire truck

(6 %) (b) Define homogenous transformation matrices to calculate the position of the hose outlet in the inertial frame. Show how the overall transformation matrix can be found. You do not need to do the matrix multiplication for full score.

Solution: To come from the attachment to the hose outlet in the chosen abstraction (task (a)), we have to rotate the system an angle θ about the z_i-axis. Hereafter, we have to rotate an angle ψ about the x_a-axis. Then we have to do a translation $l(t)$ along the y-axis. Finally, we have to rotate an angle ϕ about the x_b-axis. The overall transformation matrix can be calculated with the following homogenous transformation matrices:

$$\mathbf{T}_c^i = \mathbf{T}_a^i \mathbf{T}_{b'}^a \mathbf{T}_b^{b'} \mathbf{T}_c^b, \tag{34}$$

where

$$\mathbf{T}_a^i = \begin{bmatrix} c\theta & -s\theta & 0 & 0 \\ s\theta & c\theta & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \mathbf{T}_{b'}^a = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & c\psi & -s\psi & 0 \\ 0 & s\psi & c\psi & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \mathbf{T}_b^{b'} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & l(t) \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \mathbf{T}_c^b = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & c\phi & -s\phi & 0 \\ 0 & s\phi & c\phi & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

The overall transformation matrix is on the form

$$\mathbf{T}_c^i = \begin{pmatrix} \mathbf{R}_c^i & \mathbf{r}_c^i \\ 0 & 1 \end{pmatrix}, \tag{35}$$

where r_c^i gives the position of the hose outlet in the inertia frame.

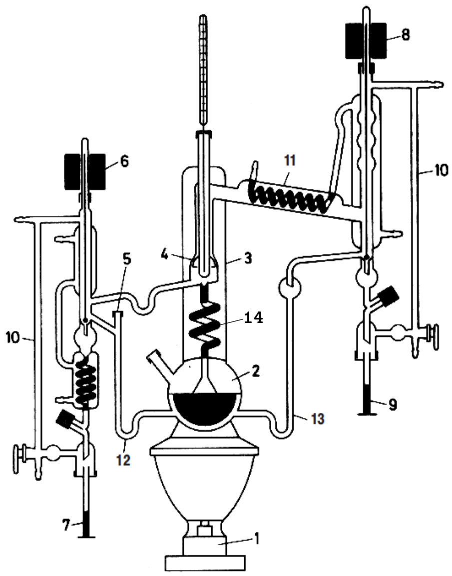
(2 %) (c) Define the position of the attachment relative to the hose outlet. Matrix multiplications are not required for full score.

> **Solution:** To find the position of the attachment relative to the hose outlet the homogenous transformation matrix can be used that describes the hose outlet relative to the inertial frame:
>
> $$\mathbf{r}_i^c = -(\mathbf{R}_c^i)^T \mathbf{r}_c^i. \tag{36}$$

Problem 5 (23 %)

In this task a measurement device used to determine the Vapor-liquid equilibrium (VLE) should be modeled (Fig 6). The VLE is is a phase equilibrium in which the liquid and vapor are in thermodynamic equilibrium. For a pure substance the VLE is determined by temperature and pressure. For composites the composition of liquid and vapor phase has to be given in addition.

In it not necessary to understand the details of the device to solve the task. Nevertheless, the basic principle of the device is to distil a composite fluid, that is, to separate the fluid by selective evaporation and condensation. A vessel containing the fluid is heated. The vapor pulls a small amount of liquid with it into the Cottrel-pump. The temperature of the vapor-liquid mixture that exits the pump is in equilibrium and measured. Afterward the two phases (liquid and vapor) are separated and recycled to the vessel. The vapor must be completely condensed before it enters the vessel, which is done in a condenser. The pressure of the device can be controlled by a vacuum-system. Moreover, samples can be taken from the recirculation pipes to determine the concentration in vapor and liquid phase.



1 Vesselheater, 2 Vessel, 3 Vacuumjacket, 4 Temperature measurement point, 5 Inputnozzle, 6 Magnetvalve - liquid sample, 7 Receiver, 8 Magnetvalve - vapor sample, 9 Receiver, 10 Vacuum pipe, 11 Condenser, 12 Circulation pipe, 13 Circulation pipe, 14 Cottrel-pump

Figure 6: Measurement device

In our model we will assume that the binary (containing two components A and B) boiling point diagram should be determined. A boiling point diagram shows the VLE for a composite. For this purpose the device is modeled as a one-tray distillation column without feed nor product outlet. The structure of the model is shown in Fig. 7. The part K_1 contains the vessel, the Cottrel-pump and the liquid reflux from the thermometer. The part K_2 represents the condenser.

In the modeling process the following assumptions are done:

- The part K_1 is heated by heat flux $\dot{Q}_H$. The part is ideally-mixed. The volume is V. The composite

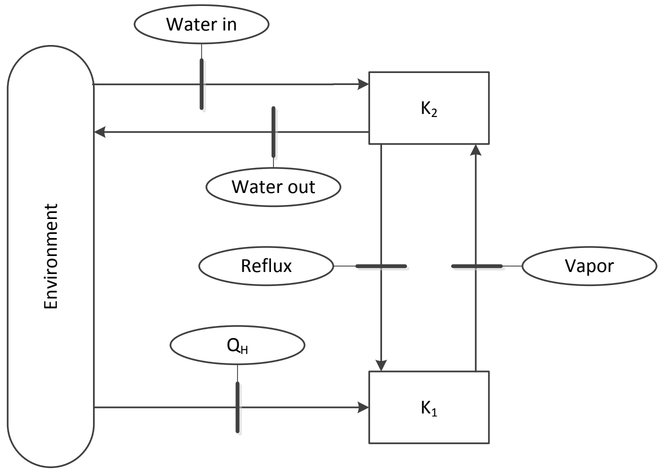


Figure 7: Model structure of measurement device.

can be described by the pressure p, the temperature T, and the mole-fraction in the liquid phase x_A, x_B and in the vapor phase y_A and y_B.

- The part K_1 is quasi-homogeneous, which means that the AB mixture is in equilibrium.
- The condenser (K_2) works as a steady-state total condenser. The outlet feed $\dot{R}$ is a saturated liquid (meaning it is exactly at boiling temperature). The mole-fractions are given by $x_{R,A}$ and $x_{R,B}$. The specific enthalpy is given by h_R. K_2 enters a known mole-flow $\dot{W}_{in}$ of cooling water with a specific mole-intensive enthalpy $h_{W,in}$. The condenser pressure is p_K.
- The vacuum-system is not modeled and the pressure p_K is a known input-variable.
- Heat losses can be neglected.
- The vapor flow into the condenser can be calculated by $\dot{V} = f(p, p_K)$. Its specific enthalpy is given by h_V.
- Potential and kinetic energies are neglected in both parts.

(6 %) (a) Derive the balance equations for the entire amount of substance n, the amount of substance of component A n_A and the internal energy U for part K_1.

Solution: The usual symbols for the variables are used. The reflux from the condenser is denoted as $\dot{R}$.

$$\frac{dn}{dt} = \dot{R} - \dot{V} \tag{37a}$$

$$\frac{dn_A}{dt} = x_{R,A}\dot{R} - y_A\dot{V} \tag{37b}$$

$$\frac{dU}{dt} = h_R\dot{R} - h_V\dot{V} + \dot{Q}_H \tag{37c}$$

To complete the model of the part K_1 "closure-relation" have to be derived. The following substance equations can be used:

$$\text{spec. mol. vapor-enthalpy of AB-mixture: } h_V = h_V(T, p, y_A, y_B), \tag{38a}$$
$$\text{spec. mol. liquid-enthalpy of AB-mixture: } h_L = h_L(T, p, x_A, x_B), \tag{38b}$$
$$\text{molar vapor-density of AB-mixture: } \rho_{m,V} = \rho_{m,V}(T, p, y_A, y_B), \tag{38c}$$
$$\text{molar liquid-density of AB-mixture: } \rho_{m,L} = \rho_{m,L}(T, p, x_A, x_B), \tag{38d}$$
$$\text{Henry's law constant of A of AB-mixture: } K_A = K_A(T, p, y_A, y_B, x_A, x_B), \tag{38e}$$
$$\text{Henry's law constant of A of AB-mixture: } K_B = K_B(T, p, y_A, y_B, x_A, x_B). \tag{38f}$$

Henry's law describes the VLE data for mixtures, where the K values are defined by

$$K_i = \frac{y_i}{x_i}. \tag{39}$$

(6 %) (b) Complete the model of K_1 with the necessary closure relations (constitutive equations and constraints). Assume, that all input molecular and energy flows as well as the vapor flow are known. *Hint:* With 12 additional equations you can complete the model (However, depending on which equations you choose it might be necessary to have more than 12 equations).

Solution: The following closure equations based on constraints and constitutive equations can be formulated in addition to the substance equations (38):

$$n = n_V + n_L \tag{40a}$$
$$n_A = n_{V,A} + n_{L,A} \tag{40b}$$
$$U = h_V n_V + h_L n_L - pV \tag{40c}$$
$$n_{V,A} = y_A n_V \tag{40d}$$
$$n_{L,A} = x_A n_L \tag{40e}$$
$$1 = y_A + y_B \tag{40f}$$
$$1 = x_A + x_B \tag{40g}$$
$$n_V = \rho_{m,V} V_V \tag{40h}$$
$$n_L = \rho_{m,L} V_L \tag{40i}$$
$$V = V_V + V_L \tag{40j}$$
$$y_A = K_A x_A \tag{40k}$$
$$y_B = K_B x_B \tag{40l}$$

(4 %) (c) Check the degrees of freedom of the equation system! How many variables have to be determined (specified as inputs or parameters) to have a well-defined equations system? Give the variables of the input vector! Assume that the volume V is the only model parameter.

Solution: The system (37) - (40) has 21 equations and 27 variables. The degrees of freedom d of the system: $d = 6$.
The input and parameter vector is:

$$\mathbf{u} = [\dot{R}, x_{R,A}, h_R, \dot{V}, \dot{Q}_H]^T \tag{41a}$$
$$\mathbf{p} = [V] \tag{41b}$$

(3 %) (d) Complete the Modelica model of the connector "port" that passes the entire mole flux J, the molar fraction y_A and the specific molar enthalpy h_j.

```
connector port

end port;
```

Solution: Instead of the in Modelica predefined variables it can also be used the `Real` variable. Important is that flow and potential variable are identified correctly.

```
connector port
 Flow MolarFlowRate J;
 MoleFraction yA;
 MolarEnthalpy hj;
end port;
```

(4 %) (e) Derive the balance equations for the total amount of substance, the amount of component A, the amount of cooling water as well as the energy of the condenser K_2.

Solution: The condenser is assumed to be in steady-state. Therefore, the following balance equations can be derived:

$$0 = \dot{V} - \dot{R} + \dot{W}_{in} - \dot{W}_{out} \tag{42a}$$

$$0 = y_A\dot{V} - x_{R,A}\dot{R} \tag{42b}$$

$$0 = \dot{W}_{in} - \dot{W}_{out} \tag{42c}$$

$$0 = h_V\dot{V} - h_R\dot{R} + h_{W,in}\dot{W}_{in} - h_{W,out}\dot{W}_{out} \tag{42d}$$