

# CHALMERS



**BOLTZMANN SOLUTION OF COUPLED NONLINEAR EQUATIONS  
FOR MOISTURE CONTENT  $w(s)$  AND TEMPERATURE  $T(s)$ ,  
 $s=x/\sqrt{4t}$ . BENCHMARK TEST I, CEN (2002).**

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Göteborg 2012

**Report 2012:8**

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REPORT NO. 2012:8, ISSN 1652-9162  
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## Contents

1. BENCHMARK TEST MODEL FOR COUPLED MOISTURE AND HEAT FLOW .....	4
2. COUPLED MOISTURE AND HEAT FLOW .....	4
2.1 Moisture and enthalpy balance equations .....	4
2.2 Liquid and vapor components .....	4
2.3 Moisture and enthalpy flows .....	4
2.4 Functional relations .....	5
2.5 Reformulation of the equations .....	6
2.6 Final equations .....	7
3. BOLTZMANN SOLUTION .....	7
3.1 Boltzmann solution .....	7
3.2 Equations for a Boltzmann solution .....	8
3.3 Four coupled ordinary differential equations .....	9
3.4 Boundary conditions for Boltzmann solution .....	10

### **Mathcad files for Benchmark Test I:**

Results: Temperature and moisture profiles for benchmark test I .....	11
Data and input functions for benchmark test I .....	20
Controls and accuracy of the solution. New Mathcad 2012.....	25

## 1. BENCHMARK TEST MODEL FOR COUPLED MOISTURE AND HEAT FLOW

There are many models for coupled moisture and heat flow in porous building materials. A question is how accurate the various models are. There is a need to compare the models with a solution with high and well documented accuracy. The model with its Mathcad files presented here tries to meet that need. It was originally presented in Dresden 2002 at a CEN meeting.

The solution is now used in a provisional European standard:

- European Provisional Standard prEN 15026, Hygrothermal Performance of Building Components and Building Elements – Assessment of Moisture Transfer by Numerical Simulation, 2005.

The presented model may be summarized in the following way:

- Highly non-linear coupled moisture and heat flow
- Highly unbalanced time scales between moisture content  $w$  and temperature  $T$
- Any functional relations for flow coefficients and state functions are easily implemented
- Directly verified accuracy from with errors in the equations below 0.03 %. See page 34.
- Implemented in Mathcad. See pages 11-44.

## 2. EQUATIONS FOR COUPLED MOISTURE AND HEAT FLOW

### 2.1 Moisture and enthalpy balance equations

We consider one-dimensional coupled moisture and heat flow in a porous building material. The mass balance for moisture and heat read:

$$\frac{\partial w}{\partial t} = -\frac{\partial g}{\partial x}, \quad x > 0, \quad t > 0. \quad (2.1)$$

$$\frac{\partial h}{\partial t} = -\frac{\partial q}{\partial x}, \quad x > 0, \quad t > 0. \quad (2.2)$$

Here,  $w$  is the moisture content ( $\text{kg}/\text{m}^3$ ),  $g$  the moisture flux ( $\text{kg}/(\text{m}^2, \text{s})$ ),  $h$  the enthalpy ( $\text{J}/\text{m}^3$ ) and  $q$  the heat and enthalpy flux ( $\text{J}/(\text{m}^2, \text{s})$ ). These quantities are functions of the coordinate  $x$  and time  $t$ .

### 2.2 Liquid and vapor components

The moisture content  $w$  in the pores is divided into a *liquid* and a *vapor* phase:

$$w = w_{\text{liq}} + w_{\text{vap}}, \quad g = g_{\text{liq}} + g_{\text{vap}}. \quad (2.3)$$

The moisture flux  $g$  is also divided into a liquid and a vapor component.

### 2.3 Moisture and enthalpy flows

The liquid flux is by assumption driven by the suction (or negative pressure)  $P_{\text{suc}}$ , which is a given function of the water content  $w$ . The corresponding hydraulic conductivity  $K(w)$  is also a given

function of  $w$ . The vapor flow is driven by the water vapor pressure  $p$  in the gas phases with a moisture-dependent flow coefficient  $\delta_p(w)$ . We assume:

$$g_{\text{liq}} = K(w) \cdot \frac{\partial P_{\text{suc}}(w)}{\partial x}, \quad g_{\text{vap}} = -\delta_p(w) \cdot \frac{\partial p}{\partial x}. \quad (2.4)$$

The energy flux  $q$  involves heat conduction and convective enthalpy flux of liquid water and water vapor:

$$q = -\lambda(w) \cdot \frac{\partial T}{\partial x} + h_{\text{liq}}(T) \cdot g_{\text{liq}} + h_{\text{vap}}(T) \cdot g_{\text{vap}}. \quad (2.5)$$

The thermal conductivity depends on the water content  $w$ . The enthalpies are essentially proportional to the temperature  $T$  ( $^{\circ}\text{C}$ ), (2.6).

#### 4.4 Functional relations

We will need relations between our various quantities. For the enthalpies we have:

$$h_{\text{solid}}(T) = c_{\text{solid}} \cdot T, \quad h_{\text{liq}}(T) = c_p \cdot T, \quad h_{\text{vap}}(T) = h_{\text{liq}}(T) + L_{\text{ev}}(T). \quad (2.6)$$

Here,  $c_{\text{solid}}$  denotes the heat capacity of the solid porous material per *unit* volume ( $\text{J}/(^{\circ}\text{C}, \text{m}^3)$ ). The heat capacity of water is  $c_p = 1000 \cdot 4184 \text{ J}/(^{\circ}\text{C}, \text{m}^3)$ , while  $L_{\text{ev}}(T)$  ( $\text{J}/\text{m}^3$ ) is the latent heat of *evaporation* of water.

The moisture content  $w$  depends on the relative humidity  $\phi$  following the *sorption* isotherm of the considered porous material:

$$w = w_{\text{sorp}}(\phi), \quad \phi = \phi_{\text{sorp}}(w), \quad \phi = \frac{p}{p_{\text{sat}}(T)}. \quad (2.7)$$

We will use the inverse to the sorption isotherm, i.e. the relative humidity  $\phi$  as a function of  $w$ .

The enthalpy of the porous material is equal to the sum of enthalpies of the solid matrix, liquid water and water vapor:

$$h = h_{\text{solid}}(T) + h_{\text{liq}}(T) \cdot w_{\text{liq}} + h_{\text{vap}}(T) \cdot w_{\text{vap}} = h_{\text{solid}}(T) + h_{\text{liq}}(T) \cdot w + L_{\text{ev}}(T) \cdot w_{\text{vap}}. \quad (2.8)$$

In the right-hand expression we have used (2.6), right.

We apply the general gas law to the water vapor in the gas part of the pore volume,  $V_{\text{pore}} - w/\rho_w$  ( $\text{m}^3/\text{m}^3$ ).

$$\frac{R \cdot (273 + T) \cdot w_{\text{vap}}}{M_w} = (V_{\text{pore}} - w/\rho_w) \cdot p. \quad (2.9)$$

Here,  $R = 8.314 \text{ J}/(\text{mole}, ^{\circ}\text{C})$  is the gas constant,  $M_w = 0.018 \text{ kg}/\text{mole}$  the molar mass of water, and  $\rho_w = 1000 \text{ kg}/\text{m}^3$  the density of liquid water.

We will use moisture content  $w$  and temperature  $T$  as basic state variables, so we need to express other variables as functions of  $w$  and  $T$ . From (2.7) we get for the water vapor pressure  $p$ :

$$p(w, T) = \phi_{\text{sorp}}(w) \cdot p_{\text{sat}}(T). \quad (2.10)$$

Combining (2.9) and (2.10), we get the water vapor content  $w_{\text{vap}}$  as function of  $w$  and  $T$

$$w_{\text{vap}}(w, T) = \frac{M_w \cdot (V_{\text{pore}} - w / \rho_w) \cdot \phi_{\text{sorp}}(w) \cdot p_{\text{sat}}(T)}{R \cdot (273 + T)}. \quad (2.11)$$

For the enthalpy we get from (2.8), right, and (2.11):

$$h(w, T) = h_{\text{solid}}(T) + h_{\text{liq}}(T) \cdot w + \frac{M_w \cdot (V_{\text{pore}} - w / \rho_w) \cdot \phi_{\text{sorp}}(w)}{R} \cdot \frac{p_{\text{sat}}(T) \cdot L_{\text{ev}}(T)}{273 + T}. \quad (2.12)$$

The input to our model for heat and moisture involves the following functions for the considered porous material:

$$K(w), \quad P_{\text{suc}}(w), \quad \delta_p(w), \quad \lambda(w), \quad w = w_{\text{sorp}}(\phi) \quad \text{or} \quad \phi = \phi_{\text{sorp}}(w). \quad (2.13)$$

These functions are a free input in the model. For water we use the liquid and vapor enthalpy, which are related to the heat of evaporation:

$$h_{\text{liq}}(T), \quad h_{\text{vap}}(T) = h_{\text{liq}}(T) + L_{\text{ev}}(T), \quad p_{\text{sat}}(T). \quad (2.14)$$

We also need an expression for the saturation water vapor pressure.

## 2.5 Reformulation of the equations

The mass conservation equation (2.1) involves the moisture flux  $g$ . We have from (2.3), right, and (2.4) and (2.10):

$$g = K(w) \cdot \frac{\partial P_{\text{suc}}(w)}{\partial x} - \delta_p(w) \cdot \frac{\partial p}{\partial x} = K(w) \cdot \frac{dP_{\text{suc}}(w)}{dw} \cdot \frac{\partial w}{\partial x} - \delta_p(w) \cdot \frac{\partial}{\partial x} (\phi_{\text{sorp}}(w) \cdot p_{\text{sat}}(T)). \quad (2.15)$$

The moisture flux has the following form:

$$g = -K_w(w, T) \cdot \frac{\partial w}{\partial x} - K_T(w, T) \cdot \frac{\partial T}{\partial x}. \quad (2.16)$$

The coefficients before the gradients become:

$$K_w(w, T) = -K(w) \cdot \frac{dP_{\text{suc}}}{dw} + \delta_p(w) \cdot \frac{d\phi_{\text{sorp}}}{dw} \cdot p_{\text{sat}}(T), \quad (2.17)$$

$$K_T(w, T) = \delta_p(w) \cdot \phi_{\text{sorp}}(w) \cdot \frac{dp_{\text{sat}}}{dT}.$$

The time derivative of the enthalpy in (2.2) may be expressed as derivatives of  $w$  and  $T$ :

$$\frac{\partial}{\partial t} [h(w, T)] = h_w(w, T) \cdot \frac{\partial w}{\partial t} + h_T(w, T) \cdot \frac{\partial T}{\partial t} = -\frac{\partial q}{\partial x}, \quad x > 0, \quad t > 0. \quad (2.18)$$

Using (2.12), we get:

$$h_w(w, T) = h_{\text{liq}}(T) + \frac{M_w}{R} \cdot \frac{d}{dw} \left[ \left( V_{\text{pore}} - \frac{w}{\rho_w} \right) \cdot \phi_{\text{sorp}}(w) \right] \cdot \frac{p_{\text{sat}}(T) \cdot L_{\text{ev}}(T)}{273 + T}, \quad (2.19)$$

$$h_T(w, T) = c_{\text{solid}} + c_w \cdot w + \frac{M_w \cdot (V_{\text{pore}} - w / \rho_w) \cdot \phi_{\text{sorp}}(w)}{R} \cdot \frac{d}{dT} \left[ \frac{p_{\text{sat}}(T) \cdot L_{\text{ev}}(T)}{273 + T} \right].$$

The enthalpy conservation equation (2.18) involves the enthalpy flux  $q$ . Using (2.5), (2.4) and (2.10), this flux may be written:

$$q = -\lambda(w) \cdot \frac{\partial T}{\partial x} + h_{\text{liq}}(T) \cdot K(w) \cdot \frac{\partial P_{\text{suc}}(w)}{\partial x} - h_{\text{vap}}(T) \cdot \delta_p(w) \cdot \frac{\partial}{\partial x} (\phi_{\text{sorp}}(w) \cdot p_{\text{sat}}(T)). \quad (2.20)$$

The enthalpy flux has the following form:

$$q = -\lambda_w(w, T) \cdot \frac{\partial w}{\partial x} - \lambda_T(w, T) \cdot \frac{\partial T}{\partial x}. \quad (2.21)$$

The coefficients before the gradients become:

$$\begin{aligned} \lambda_w(w, T) &= -h_{\text{liq}}(T) \cdot K(w) \cdot \frac{dP_{\text{suc}}}{dw} + h_{\text{vap}}(T) \cdot \delta_p(w) \cdot \frac{d\phi_{\text{sorp}}}{dw} \cdot p_{\text{sat}}(T), \\ \lambda_T(w, T) &= \lambda(w) + h_{\text{vap}}(T) \cdot \delta_p(w) \cdot \phi_{\text{sorp}}(w) \cdot \frac{dp_{\text{sat}}}{dT}. \end{aligned} \quad (2.22)$$

## 2.6 Final equations

The final equations for the fluxes are now from (2.16) and (2.21):

$$g = -K_w(w, T) \cdot \frac{\partial w}{\partial x} - K_T(w, T) \cdot \frac{\partial T}{\partial x}, \quad (2.23)$$

$$q = -\lambda_w(w, T) \cdot \frac{\partial w}{\partial x} - \lambda_T(w, T) \cdot \frac{\partial T}{\partial x}, \quad x \geq 0, \quad t \geq 0. \quad (2.24)$$

The conservation equations for moisture and enthalpy become from from (2.1) and (2.18):

$$\frac{\partial w}{\partial t} = -\frac{\partial g}{\partial x} = \frac{\partial}{\partial x} \left[ K_w(w, T) \cdot \frac{\partial w}{\partial x} + K_T(w, T) \cdot \frac{\partial T}{\partial x} \right], \quad x > 0, \quad t > 0. \quad (2.25)$$

$$h_w(w, T) \cdot \frac{\partial w}{\partial t} + h_T(w, T) \cdot \frac{\partial T}{\partial t} = -\frac{\partial q}{\partial x} = \frac{\partial}{\partial x} \left[ \lambda_w(w, T) \cdot \frac{\partial w}{\partial x} + \lambda_T(w, T) \cdot \frac{\partial T}{\partial x} \right]. \quad (2.26)$$

## 3. BOLTZMANN SOLUTION

Boltzmann solutions are applicable to certain diffusive partial differential equations in a semi-infinite region. Spatial derivatives of the second order and time derivatives of the first order occur in the diffusive partial differential equations. In particular cases we may get solutions for a single variable  $s = x / \sqrt{4t}$ . The partial differential equations in  $x$  and  $t$  become ordinary differential equations in the variable  $s$ . Only problems for very special boundary and initial conditions may be solved.

### 3.1 Boltzmann solution

We consider a step-response problem in a semi-infinite slab. The *initial* moisture content and temperature at  $t = 0$  are constant through the slab, and the *boundary* moisture content and temperature at  $x = 0$  are constant in time:

$$\begin{aligned}
w(x,0) &= w_{\text{in}}, & T(x,0) &= T_{\text{in}}, & 0 < x < \infty, \\
w(0,t) &= w_b, & T(0,t) &= T_b, & 0 < t < \infty.
\end{aligned} \tag{3.1}$$

Here,  $w_{\text{in}}$ ,  $T_{\text{in}}$ ,  $w_b$  and  $T_b$  are any prescribed numbers.

We seek a solution of the following type:

$$w(x,t) = \tilde{w}(s), \quad T(x,t) = \tilde{T}(s), \quad s = \frac{x}{\sqrt{4 \cdot t}}. \tag{3.2}$$

### 3.2 Equations for a Boltzmann solution

The solution of the type (3.2) shall satisfy the equations (2.23)-(2.26). We need the partial derivatives of the Boltzmann coordinate  $s = s(x,t)$ :

$$s = \frac{x}{\sqrt{4 \cdot t}} \Rightarrow \frac{\partial s}{\partial x} = \frac{1}{\sqrt{4 \cdot t}}, \quad \frac{\partial s}{\partial t} = \frac{x}{\sqrt{4 \cdot t}} \cdot \frac{-1}{2t} = \frac{-s}{2t}. \tag{3.3}$$

The moisture flux (2.23) becomes:

$$g(x,t) = -K_w(\tilde{w}, \tilde{T}) \cdot \frac{d\tilde{w}}{ds} \cdot \frac{1}{\sqrt{4t}} - K_T(\tilde{w}, \tilde{T}) \cdot \frac{d\tilde{T}}{ds} \cdot \frac{1}{\sqrt{4t}}. \tag{3.4}$$

The moisture flux becomes equal to a ‘‘Boltzmann moisture flux’’  $\tilde{g}(s)$  multiplied by a time factor:

$$g(x,t) = \tilde{g}(s) \cdot \frac{1}{\sqrt{4t}}, \quad \tilde{g}(s) = -K_w(\tilde{w}, \tilde{T}) \cdot \frac{d\tilde{w}}{ds} - K_T(\tilde{w}, \tilde{T}) \cdot \frac{d\tilde{T}}{ds}. \tag{3.5}$$

The enthalpy flux (2.24) becomes:

$$q(x,t) = -\lambda_w(\tilde{w}, \tilde{T}) \cdot \frac{d\tilde{w}}{ds} \cdot \frac{1}{\sqrt{4t}} - \lambda_T(\tilde{w}, \tilde{T}) \cdot \frac{d\tilde{T}}{ds} \cdot \frac{1}{\sqrt{4t}}. \tag{3.6}$$

The enthalpy flux becomes equal to a ‘‘Boltzmann enthalpy flux’’  $\tilde{q}(s)$  multiplied by our time factor:

$$q(x,t) = \tilde{q}(s) \cdot \frac{1}{\sqrt{4t}}, \quad \tilde{q}(s) = -\lambda_w(\tilde{w}, \tilde{T}) \cdot \frac{d\tilde{w}}{ds} - \lambda_T(\tilde{w}, \tilde{T}) \cdot \frac{d\tilde{T}}{ds}. \tag{3.7}$$

The moisture conservation equation (2.1) becomes with the use of (3.3) and (3.5), left:

$$\frac{\partial w}{\partial t} = -\frac{\partial g}{\partial x} \Rightarrow \frac{d\tilde{w}}{ds} \cdot \frac{-s}{2t} = -\frac{\partial}{\partial x} \left( \frac{\tilde{g}(s)}{\sqrt{4 \cdot t}} \right) = -\frac{d\tilde{g}}{ds} \cdot \frac{1}{\sqrt{4 \cdot t}} \cdot \frac{1}{\sqrt{4 \cdot t}}. \tag{3.8}$$

The time factor cancels and we get:

$$2s \cdot \frac{d\tilde{w}}{ds} = \frac{d\tilde{q}}{ds}, \quad 0 \leq s < \infty. \tag{3.9}$$

The enthalpy conservation equation (2.18) becomes with the use of (3.3) and (3.7), left:

$$h_w(\tilde{w}, \tilde{T}) \cdot \frac{d\tilde{w}}{ds} \cdot \frac{-s}{2t} + h_T(\tilde{w}, \tilde{T}) \cdot \frac{d\tilde{T}}{ds} \cdot \frac{-s}{2t} = -\frac{d\tilde{q}}{ds} \cdot \frac{1}{\sqrt{4 \cdot t}} \cdot \frac{1}{\sqrt{4 \cdot t}}. \tag{3.10}$$



The time factor cancels and we get:

$$2s \cdot \left[ h_w(\tilde{w}, \tilde{T}) \cdot \frac{d\tilde{w}}{ds} + h_T(\tilde{w}, \tilde{T}) \cdot \frac{d\tilde{T}}{ds} \right] = \frac{d\tilde{q}}{ds}, \quad 0 \leq s < \infty. \quad (3.11)$$

### 3.3 Four coupled ordinary differential equations

We have obtained four coupled first-order ordinary differential equations:

$$\tilde{g}(s) = -K_w(\tilde{w}, \tilde{T}) \cdot \frac{d\tilde{w}}{ds} - K_T(\tilde{w}, \tilde{T}) \cdot \frac{d\tilde{T}}{ds} \quad (3.12)$$

$$\tilde{q}(s) = -\lambda_w(\tilde{w}, \tilde{T}) \cdot \frac{d\tilde{w}}{ds} - \lambda_T(\tilde{w}, \tilde{T}) \cdot \frac{d\tilde{T}}{ds} \quad (3.13)$$

$$2s \cdot \frac{d\tilde{w}}{ds} = \frac{d\tilde{g}}{ds}, \quad 0 \leq s < \infty. \quad (3.14)$$

$$2s \cdot \left[ h_w(\tilde{w}, \tilde{T}) \cdot \frac{d\tilde{w}}{ds} + h_T(\tilde{w}, \tilde{T}) \cdot \frac{d\tilde{T}}{ds} \right] = \frac{d\tilde{q}}{ds}, \quad 0 \leq s < \infty. \quad (3.15)$$

The first two equations (3.12)-(3.13) may be written as a matrix relation:

$$\begin{pmatrix} \tilde{g}(s) \\ \tilde{q}(s) \end{pmatrix} = - \begin{pmatrix} K_w & K_T \\ \lambda_w & \lambda_T \end{pmatrix} \cdot \frac{d}{ds} \begin{pmatrix} \tilde{w}(s) \\ \tilde{T}(s) \end{pmatrix}. \quad (3.16)$$

Using the inverse 2x2 matrix, we get:

$$\frac{d}{ds} \begin{pmatrix} \tilde{w}(s) \\ \tilde{T}(s) \end{pmatrix} = \frac{-1}{\text{Det}_{K\lambda}} \cdot \begin{pmatrix} \lambda_T & -K_T \\ -\lambda_w & K_w \end{pmatrix} \cdot \begin{pmatrix} \tilde{g}(s) \\ \tilde{q}(s) \end{pmatrix}, \quad \text{Det}_{K\lambda} = K_w \lambda_T - K_T \lambda_w. \quad (3.17)$$

The other two equations (3.14)-(3.15) may also be written as a matrix relation:

$$\frac{d}{ds} \begin{pmatrix} \tilde{g}(s) \\ \tilde{q}(s) \end{pmatrix} = 2s \cdot \begin{pmatrix} 1 & 0 \\ h_w & h_T \end{pmatrix} \cdot \frac{d}{ds} \begin{pmatrix} \tilde{w}(s) \\ \tilde{T}(s) \end{pmatrix} = \frac{-2s}{\text{Det}_{K\lambda}} \cdot \begin{pmatrix} 1 & 0 \\ h_w & h_T \end{pmatrix} \cdot \begin{pmatrix} \lambda_T & -K_T \\ -\lambda_w & K_w \end{pmatrix} \cdot \begin{pmatrix} \tilde{g}(s) \\ \tilde{q}(s) \end{pmatrix}. \quad (3.18)$$

In the right-hand matrix expression, (3.17) is inserted.

From (3.17)-(3.18) we have obtained the following four coupled ordinary differential equations:

$$\begin{cases} \frac{d\tilde{w}}{ds} = -\frac{\lambda_T}{\text{Det}_{K\lambda}} \cdot \tilde{g}(s) + \frac{K_T}{\text{Det}_{K\lambda}} \cdot \tilde{q}(s) \\ \frac{d\tilde{T}}{ds} = \frac{\lambda_w}{\text{Det}_{K\lambda}} \cdot \tilde{g}(s) - \frac{K_w}{\text{Det}_{K\lambda}} \cdot \tilde{q}(s) \\ \frac{d\tilde{g}}{ds} = -2s \cdot \frac{\lambda_T}{\text{Det}_{K\lambda}} \cdot \tilde{g}(s) + 2s \cdot \frac{K_T}{\text{Det}_{K\lambda}} \cdot \tilde{q}(s) \\ \frac{d\tilde{q}}{ds} = -2s \cdot \frac{h_w \lambda_T - h_T \lambda_w}{\text{Det}_{K\lambda}} \cdot \tilde{g}(s) + 2s \cdot \frac{h_w K_T - h_T K_w}{\text{Det}_{K\lambda}} \cdot \tilde{q}(s) \end{cases} \quad 0 \leq s < \infty. \quad (3.19)$$

Here, we use the following functions, which are defined in (2.17), (2.22), (2.19) and (3.17), right:

$$\begin{aligned}
K_w &= K_w(\tilde{w}, \tilde{T}), & K_T &= K_T(\tilde{w}, \tilde{T}), & \lambda_w &= \lambda_w(\tilde{w}, \tilde{T}), \\
\lambda_T &= \lambda_T(\tilde{w}, \tilde{T}), & h_w &= h_w(\tilde{w}, \tilde{T}), & h_T &= h_T(\tilde{w}, \tilde{T}), \\
\text{Det}_{K\lambda} &= \text{Det}_{K\lambda}(\tilde{w}, \tilde{T}) = K_w(\tilde{w}, \tilde{T}) \cdot \lambda_T(\tilde{w}, \tilde{T}) - K_T(\tilde{w}, \tilde{T}) \cdot \lambda_w(\tilde{w}, \tilde{T}).
\end{aligned} \tag{3.20}$$

The equation system (3.19) is of the following type:

$$\frac{d}{ds} \begin{pmatrix} \tilde{w}(s) \\ \tilde{T}(s) \\ \tilde{g}(s) \\ \tilde{q}(s) \end{pmatrix} = \begin{pmatrix} F_w(s, \tilde{w}, \tilde{T}, \tilde{g}, \tilde{q}) \\ F_T(s, \tilde{w}, \tilde{T}, \tilde{g}, \tilde{q}) \\ F_g(s, \tilde{w}, \tilde{T}, \tilde{g}, \tilde{q}) \\ F_q(s, \tilde{w}, \tilde{T}, \tilde{g}, \tilde{q}) \end{pmatrix}, \quad 0 \leq s < \infty. \tag{3.21}$$

Here, the right-hand expressions  $F_{\text{sub}}(s, \tilde{w}, \tilde{T}, \tilde{g}, \tilde{q})$ , sub =  $w, T, g$  and  $q$ , are given functions of  $s$  and the four state functions. This kind of coupled ordinary differential equations is easily solved with high accuracy in mathematical computer programs such as Mathcad. We need four boundary conditions to have a solution.

### 3.4 Boundary conditions for Boltzmann solution

The initial conditions (3.1), upper line, and the boundary condition (3.1), lower line, correspond to infinite  $s$  and to  $s = 0$ :

$$\begin{aligned}
t \rightarrow 0, \quad x > 0 &\Rightarrow s \rightarrow \infty; & x = 0, \quad t > 0 &\Rightarrow s = 0: \\
\tilde{w}(\infty) = w_{\text{in}}, & \quad \tilde{T}(\infty) = T_{\text{in}}, & \tilde{w}(0) = w_{\text{b}}, & \quad \tilde{T}(0) = T_{\text{b}}.
\end{aligned} \tag{3.22}$$

The moisture content and the temperature at  $s = 0$  are prescribed. We have to choose the moisture and heat flux at  $s = 0$  so that the prescribed initial values are obtained:

$$\tilde{g}(0) \text{ and } \tilde{q}(0) \text{ to be chosen so that } \tilde{w}(\infty) = w_{\text{in}} \text{ and } \tilde{T}(\infty) = T_{\text{in}}. \tag{3.23}$$

**Boltzmann solution of coupled nonlinear equations for moisture content  $w(s)$  and temperature  $T(s)$ ,  $s=x/\text{root}(4t)$ . Benchmark test I, CEN. Dresden 2002.**

J. Claesson

**Input data.**

Initial and boundary conditions

$$\phi_{in} := 0.5 \quad T_{in} := 20 \quad \phi_b := 0.95 \quad T_b := 30$$

**Constants**

$$T_{ref} := 20 \quad T_{Kref} := 273.15 + T_{ref} \quad \rho_w := 1000 \quad \underline{R}_w := 8.314 \quad M_w := 0.018$$

**Sorption isotherm.**

$$w\phi(\phi) := \frac{146}{\left[ 1 + \left( -8 \cdot 10^{-8} \cdot \frac{R \cdot T_{Kref} \cdot \rho_w}{M_w} \cdot \ln(\phi) \right)^{1.6} \right]^{0.375}} \quad \phi_w(w) := e^{\frac{-M_w}{R \cdot T_{Kref} \cdot \rho_w} \cdot 0.125 \cdot 10^8 \cdot \left[ \left( \frac{146}{w} \right)^{0.375} - 1 \right]^{0.625}}$$

**Initial and boundary moisture content:**

$$w_{in} := w\phi(\phi_{in}) \quad w_b := w\phi(\phi_b) \quad w_{in} = 42.922 \quad w_b = 129.021$$

**Water retention curve.**

$$wP_{suc}(P_{suc}) := \frac{146}{\left[ 1 + \left( 8 \cdot 10^{-8} \cdot P_{suc} \right)^{1.6} \right]^{0.375}} \quad P_{suc}w(w) := 0.125 \cdot 10^8 \cdot \left[ \left( \frac{146}{w} \right)^{0.375} - 1 \right]^{0.625}$$

**Vapor diffusion coefficient.**

$$\delta p(w) := \frac{M_w}{R \cdot T_{Kref}} \cdot \frac{26.1 \cdot 10^{-6}}{200} \cdot \frac{1 - \frac{w}{146}}{0.503 \cdot \left( 1 - \frac{w}{146} \right)^2 + 0.497}$$

**Liquid water permeability.**

$$\underline{K}(w) := e^{-39.2619 + 0.0704 \cdot (w-73) - 1.742 \cdot 10^{-4} \cdot (w-73)^2 - 2.7953 \cdot 10^{-6} \cdot (w-73)^3 - 1.1566 \cdot 10^{-7} \cdot (w-73)^4 + 2.5969 \cdot 10^{-9} \cdot (w-73)^5}$$

**Formula for  $p_{sat}(T)$ .**

$$E_{psat}(T) := \frac{19.625 \cdot T}{270.1 + T} - \frac{0.00463 \cdot T^2}{142.15 + T} \quad p_{sat}(T) := 610.8 \cdot e^{E_{psat}(T)}$$

**Heat of evaporation.**

$$Lev(T) := 10^6 \cdot \left[ 2.5016 - \frac{T}{422} - \left( \frac{T}{342} \right)^4 \right]$$

**Heat content (enthalpy) of water and water vapor.**

$$hl(T) := 4184 \cdot T \quad hv(T) := hl(T) + Lev(T)$$

Thermal conductivity.

$$\lambda(w) := 1.5 + 0.0158 \cdot w$$

Water vapor content

$$V_p := 0.146 \quad (\text{pore volume}) \quad w_{\text{vap}}(w, T) := \left( V_p - \frac{w}{\rho_w} \right) \cdot \phi_w(w) \cdot \frac{M_w \cdot p_{\text{sat}}(T)}{R \cdot (273.15 + T)}$$

Total energy (enthalpy)

$$h(w, T) := 1.824 \cdot 10^6 \cdot T + h_l(T) \cdot w + \text{Lev}(T) \cdot w_{\text{vap}}(w, T) \quad (\text{only used for control})$$

Capacity functions (derivatives of  $h(w, T)$ ).

$$h_w(w, T) := h_l(T) + \text{Lev}(T) \cdot \frac{M_w \cdot p_{\text{sat}}(T)}{R \cdot (273.15 + T)} \cdot \left[ -\frac{\phi_w(w)}{\rho_w} + \left( V_p - \frac{w}{\rho_w} \right) \cdot \left( \frac{d}{dw} \phi_w(w) \right) \right]$$

$$h_T(w, T) := 1.824 \cdot 10^6 + 4184 \cdot w + \left( V_p - \frac{w}{\rho_w} \right) \cdot \frac{\phi_w(w) \cdot M_w}{R} \cdot \frac{d}{dT} \left( \frac{\text{Lev}(T) \cdot p_{\text{sat}}(T)}{273.15 + T} \right)$$

### Auxilliary functions.

Functions for flow coefficients:

$$K_w(w, T) := K(w) \cdot \frac{d}{dw} (-P_{\text{sucw}}(w)) + p_{\text{sat}}(T) \cdot \delta p(w) \cdot \frac{d}{dw} (\phi_w(w))$$

$$\lambda_w(w, T) := -h_l(T) \cdot K(w) \cdot \frac{d}{dw} (P_{\text{sucw}}(w)) + h_v(T) \cdot p_{\text{sat}}(T) \cdot \delta p(w) \cdot \frac{d}{dw} (\phi_w(w))$$

$$K_T(w, T) := \delta p(w) \cdot \phi_w(w) \cdot \frac{d}{dT} p_{\text{sat}}(T) \quad \lambda_T(w, T) := \lambda(w) + h_v(T) \cdot \delta p(w) \cdot \phi_w(w) \cdot \frac{d}{dT} p_{\text{sat}}(T)$$

Determinant and R-functions:

$$\text{DetK}\lambda(w, T) := K_w(w, T) \cdot \lambda_T(w, T) - K_T(w, T) \cdot \lambda_w(w, T)$$

$$R_1(w, T) := \frac{\lambda_T(w, T)}{\text{DetK}\lambda(w, T)} \quad R_2(w, T) := \frac{-K_T(w, T)}{\text{DetK}\lambda(w, T)} \quad R_3(w, T) := \frac{-\lambda_w(w, T)}{\text{DetK}\lambda(w, T)}$$

$$R_4(w, T) := \frac{K_w(w, T)}{\text{DetK}\lambda(w, T)} \quad R_5(w, T) := \frac{\lambda_T(w, T)}{\text{DetK}\lambda(w, T)} \quad R_6(w, T) := \frac{-K_T(w, T)}{\text{DetK}\lambda(w, T)}$$

$$R_7(w, T) := \frac{h_w(w, T) \cdot \lambda_T(w, T) - h_T(w, T) \cdot \lambda_w(w, T)}{\text{DetK}\lambda(w, T)} \quad R_8(w, T) := \frac{-h_w(w, T) \cdot K_T(w, T) + h_T(w, T) \cdot K_w(w, T)}{\text{DetK}\lambda(w, T)}$$

### Calculations.

Estimates of moisture and temperature penetration depths.

$$L_{\text{pen}w} := \sqrt{K_w(w_b, T_b)} \quad L_{\text{pen}T} := \sqrt{\frac{\lambda_T(w_b, T_b)}{h_T(w_b, T_b)}} \quad L_{\text{pen}w} = 8.469 \times 10^{-6} \quad L_{\text{pen}T} = 1.224 \times 10^{-3}$$

Coupled differential equations for w(s), T(s), g(s) and q(s).

$$D(s, y) := (-1) \cdot \begin{bmatrix} R_1(y_0, y_1) \cdot y_2 + R_2(y_0, y_1) \cdot y_3 \\ R_3(y_0, y_1) \cdot y_2 + R_4(y_0, y_1) \cdot y_3 \\ 2 \cdot s \cdot (R_5(y_0, y_1) \cdot y_2 + R_6(y_0, y_1) \cdot y_3) \\ 2 \cdot s \cdot (R_7(y_0, y_1) \cdot y_2 + R_8(y_0, y_1) \cdot y_3) \end{bmatrix} \quad \begin{array}{l} (y.0=w) \\ (y.1=T) \\ (y.2=g) \\ (y.3=q) \end{array}$$

Estimate of fluxes at s=0.

$$gbinit := Kw(wb, Tb) \cdot \frac{wb - win}{Lpenw} + KT(wb, Tb) \cdot \frac{Tb - Tin}{LpenT} \quad qbinit := \lambda w(wb, Tb) \cdot \frac{wb - win}{Lpenw} + \lambda T(wb, Tb) \cdot \frac{Tb - Tin}{LpenT}$$

$$gbinit = 7.296 \times 10^{-4} \quad qbinit = 2.907 \times 10^4$$

### Solution in moisture penetration region.

Range:  $smax := 3 \cdot Lpenw \quad smax = 2.541 \times 10^{-5}$

Values at s=0:  $y_0 := wb \quad y_1 := Tb$

Iterativ choice of fluxes g(0) and q(0).

$$y_2 := 0.8131 \cdot gbinit \quad y_3 := 0.815 \cdot qbinit$$

$$y = \begin{pmatrix} 129.021 \\ 30 \\ 5.932 \times 10^{-4} \\ 2.369 \times 10^4 \end{pmatrix}$$

Runge-Kutta solver:  $N := 100 \quad Z := rkfixed(y, 0, smax, N, D)$

$$i := 0..N \quad w_i := Z_{i,0} \quad T_i := Z_{i,1} \quad g_i := Z_{i,2} \quad q_i := Z_{i,3}$$

Iterations for choice of g(0) to get w(smax)=win:

$$w_N = 42.919 \quad win = 42.922$$

### Continued solution for thermal penetration region.

Constant moisture content:  $winf := w_N \quad winf = 42.919$

Range:  $smax1 := 3 \cdot LpenT \quad smax1 = 3.671 \times 10^{-3}$  Initial values:  $y1_0 := T_N \quad y1_1 := q_N$

Differential equations for T(s) and q(s) for constant moisture content:

$$D1(s1, y1) := (-1) \cdot \begin{pmatrix} \frac{1}{\lambda T(winf, y1_0)} \cdot y1_1 \\ 2 \cdot s1 \cdot \frac{hT(winf, y1_0)}{\lambda T(winf, y1_0)} \cdot y1_1 \end{pmatrix} \quad \begin{array}{l} (y1.0=T) \\ (y1.1=q) \end{array} \quad y1 = \begin{pmatrix} 29.743 \\ 2.36 \times 10^4 \end{pmatrix}$$

Runge-Kutta solver:  $N1 := 100 \quad Z1 := rkfixed(y1, smax, smax1, N1, D1)$

$$i := 0..N1 \quad s1_i := Z1_{i,0} \quad T1_i := Z1_{i,1} \quad q1_i := Z1_{i,2}$$

Iterations for choice of q(0) to get T(smax1)=Tin:

$$T1_{N1} = 20.001 \quad Tin = 20$$

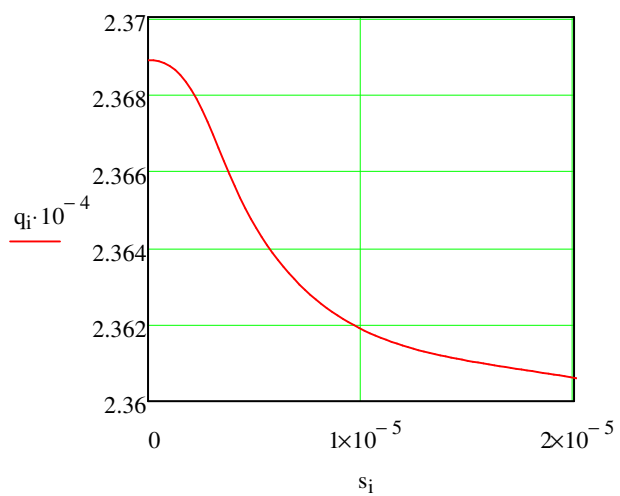
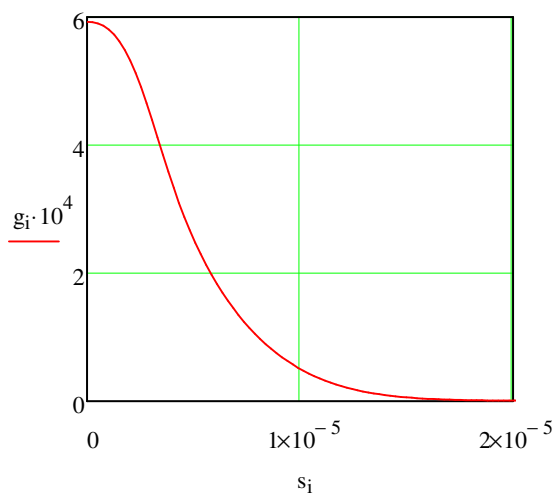
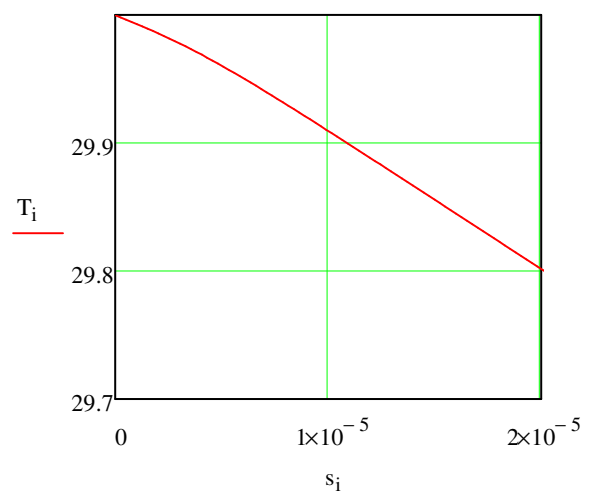
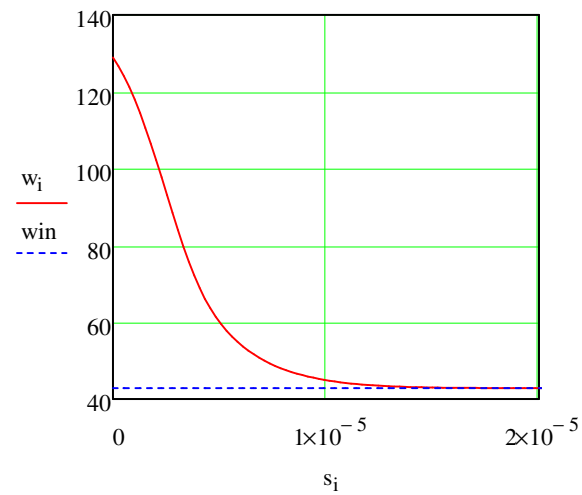
**Diagrams for the result.**

$$i := N + 1..N + N1 \quad s_i := s1_{i-N} \quad w_i := winf \quad T_i := T1_{i-N} \quad g_i := 0 \quad q_i := q1_{i-N}$$

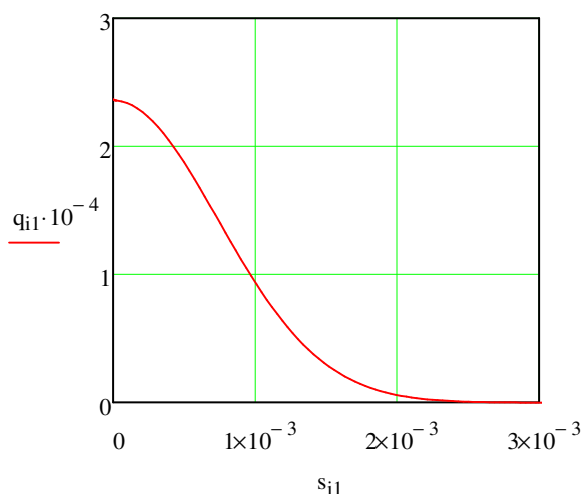
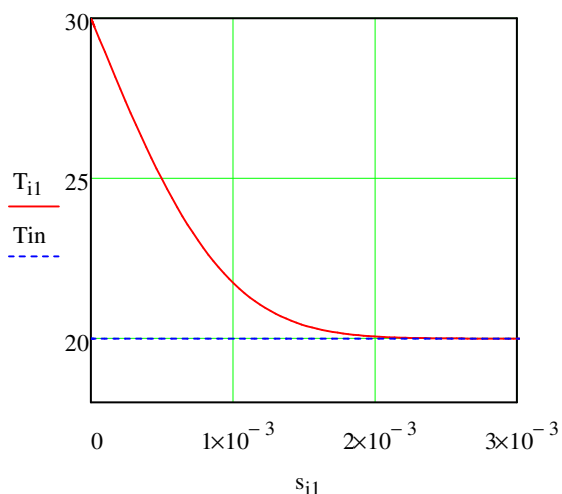
$$i := 0..N \quad i1 := 0..N + N1$$

**Benchmark test I, CEN.**

Moisture penetration region

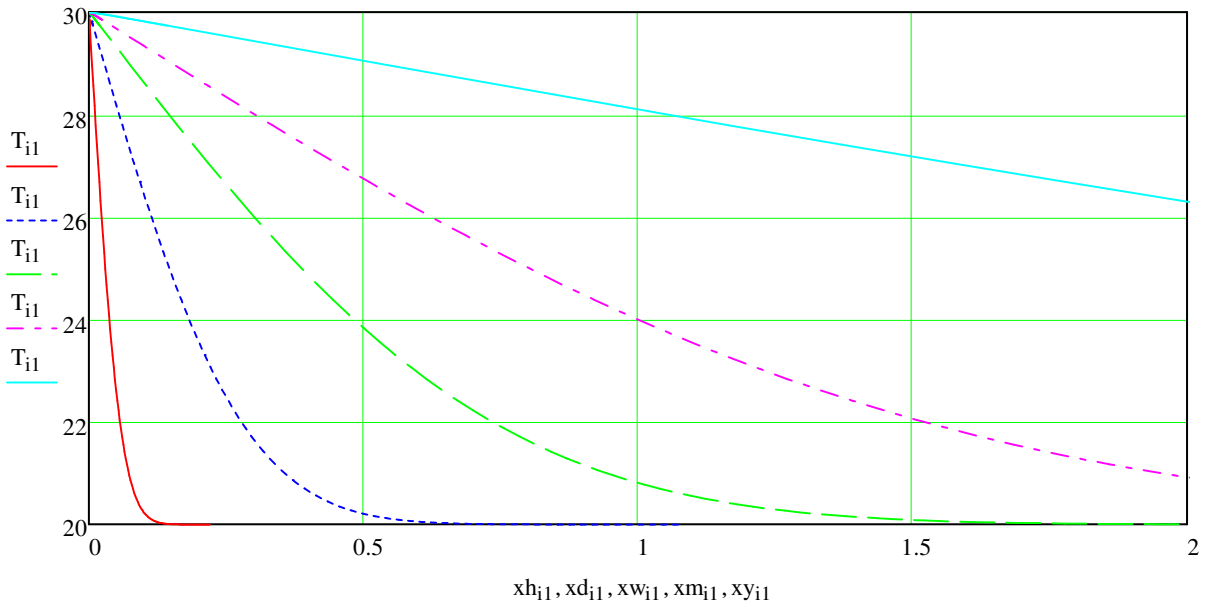
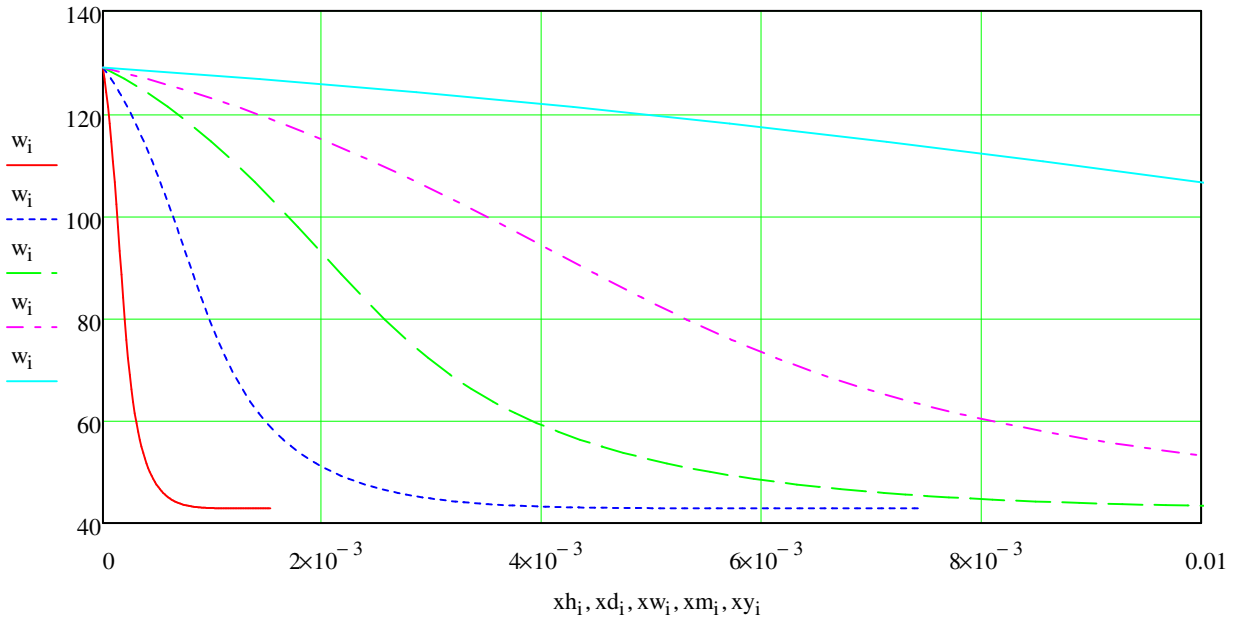


Thermal penetration region

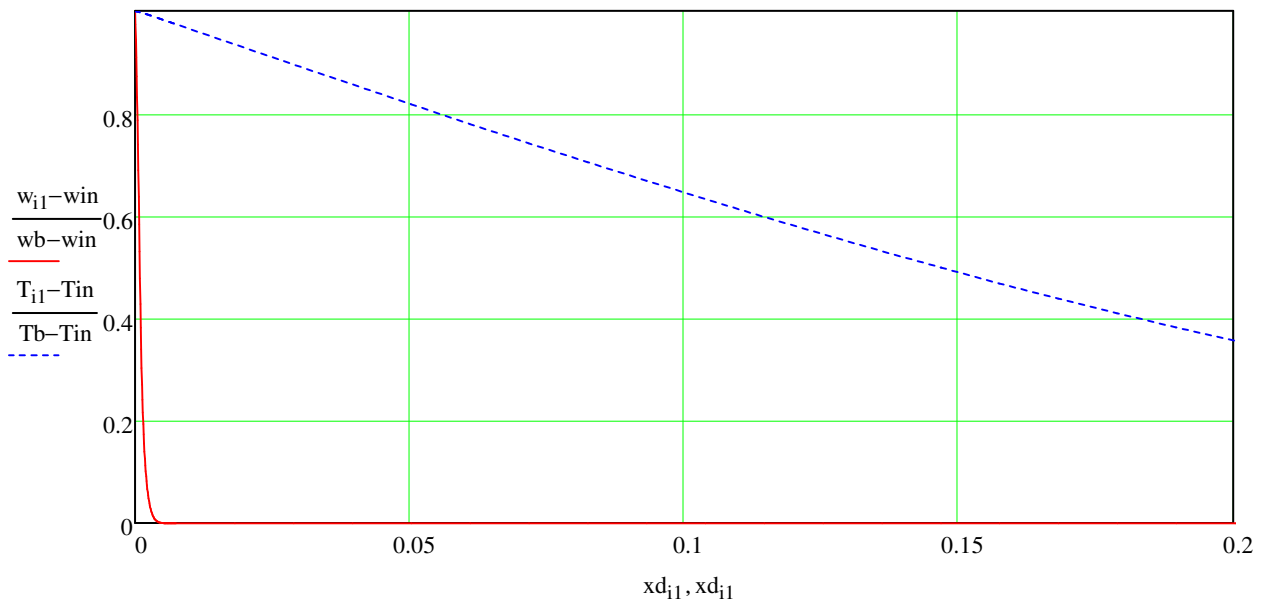


Functions of x for a few t.

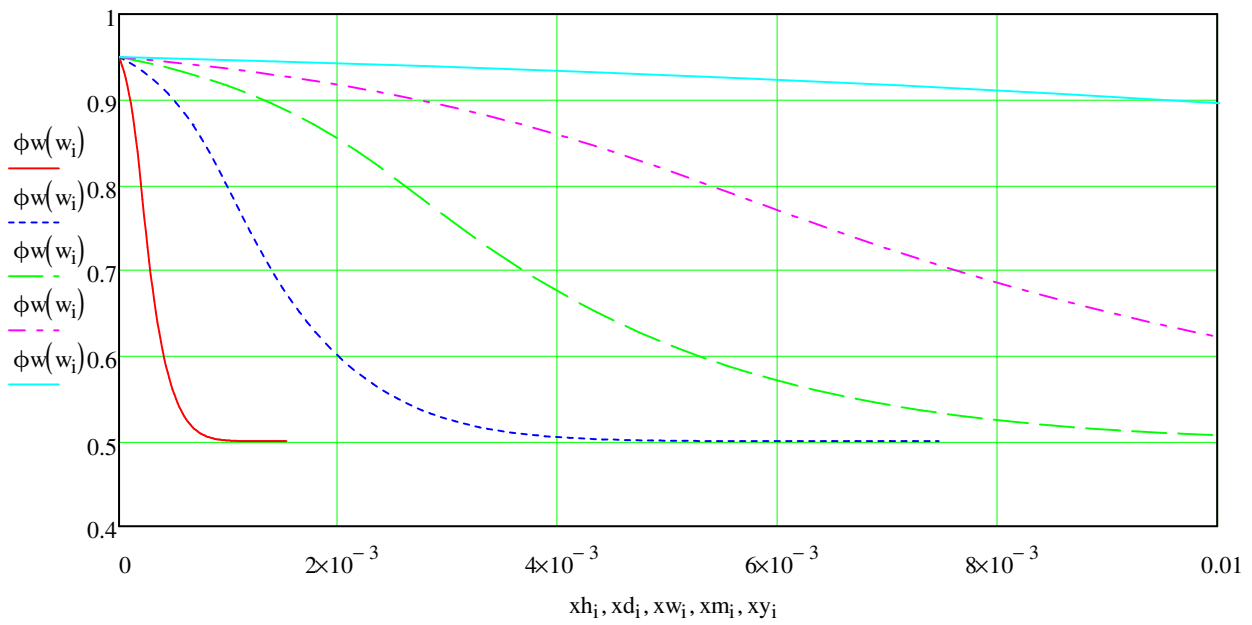
$$\begin{array}{ccccc}
 x_h := \sqrt{3600} \cdot s & x_d := \sqrt{24 \cdot 3600} \cdot s & x_w := \sqrt{7 \cdot 24 \cdot 3600} \cdot s & x_m := \sqrt{30 \cdot 24 \cdot 3600} \cdot s & x_y := \sqrt{365 \cdot 24 \cdot 3600} \cdot s \\
 \text{(hour)} & \text{(day)} & \text{(week)} & \text{(month)} & \text{(year)}
 \end{array}$$



Moisture and temperature in the same diagram (t=24 h).



Relative humidity.





$$wf(sf) := \begin{cases} \text{linterp}(s, w, sf) \\ w_{200} \text{ if } sf \geq s_{200} \end{cases} \quad Tf(sf) := \begin{cases} \text{linterp}(s, T, sf) \\ T_{200} \text{ if } sf \geq s_{200} \end{cases} \quad s_{200} = 3.671 \times 10^{-3}$$

$$I := 10 \quad i := 0..I \quad x_i := \frac{i}{I} \cdot 0.1$$

$$wh_i := wf\left(\frac{x_i}{\sqrt{4 \cdot 3600}}\right) \quad wd_i := wf\left(\frac{x_i}{\sqrt{4 \cdot 3600 \cdot 24}}\right) \quad ww_i := wf\left(\frac{x_i}{\sqrt{4 \cdot 3600 \cdot 24 \cdot 7}}\right)$$

$$wm_i := wf\left(\frac{x_i}{\sqrt{4 \cdot 3600 \cdot 24 \cdot 30}}\right) \quad wy_i := wf\left(\frac{x_i}{\sqrt{4 \cdot 3600 \cdot 24 \cdot 365}}\right)$$

 $x =$ 

	0
0	0
1	0.01
2	0.02
3	0.03
4	0.04
5	0.05
6	0.06
7	0.07
8	0.08
9	0.09
10	0.1

 $wh =$ 

	0
0	129.021
1	42.919
2	42.919
3	42.919
4	42.919
5	42.919
6	42.919
7	42.919
8	42.919
9	42.919
10	42.919

 $wd =$ 

	0
0	129.021
1	42.965
2	42.919
3	42.919
4	42.919
5	42.919
6	42.919
7	42.919
8	42.919
9	42.919
10	42.919

 $ww =$ 

	0
0	129.021
1	52.391
2	43.439
3	42.929
4	42.919
5	42.919
6	42.919
7	42.919
8	42.919
9	42.919
10	42.919

 $wm =$ 

	0
0	129.021
1	83.109
2	53.288
3	45.732
4	43.569
5	43.035
6	42.934
7	42.921
8	42.919
9	42.919
10	42.919

 $wy =$ 

	0
0	129.021
1	119.668
2	106.561
3	90.833
4	75.747
5	64.901
6	57.823
7	53.197
8	50.025
9	47.832
10	46.281

$$\text{Matw} := \text{augment}(x, wh, wd, ww, wm, wy)$$

$$I := 10 \quad i := 0..I \quad x_i := \frac{i}{I} \cdot 5$$

$$Th_i := Tf\left(\frac{x_i}{\sqrt{4 \cdot 3600}}\right) \quad Td_i := Tf\left(\frac{x_i}{\sqrt{4 \cdot 3600 \cdot 24}}\right) \quad Tw_i := Tf\left(\frac{x_i}{\sqrt{4 \cdot 3600 \cdot 24 \cdot 7}}\right)$$

$$Tm_i := Tf\left(\frac{x_i}{\sqrt{4 \cdot 3600 \cdot 24 \cdot 30}}\right) \quad Ty_i := Tf\left(\frac{x_i}{\sqrt{4 \cdot 3600 \cdot 24 \cdot 365}}\right)$$

 $x =$ 

	0
0	0
1	0.5
2	1
3	1.5
4	2
5	2.5
6	3
7	3.5
8	4
9	4.5
10	5

 $Th =$ 

	0
0	30
1	20.001
2	20.001
3	20.001
4	20.001
5	20.001
6	20.001
7	20.001
8	20.001
9	20.001
10	20.001

 $Td =$ 

	0
0	30
1	22.494
2	20.212
3	20.007
4	20.001
5	20.001
6	20.001
7	20.001
8	20.001
9	20.001
10	20.001

 $Tw =$ 

	0
0	30
1	26.641
2	23.84
3	21.914
4	20.815
5	20.295
6	20.09
7	20.024
8	20.006
9	20.002
10	20.001

 $Tm =$ 

	0
0	30
1	28.348
2	26.749
3	25.286
4	24.005
5	22.931
6	22.069
7	21.408
8	20.924
9	20.583
10	20.354

 $Ty =$ 

	0
0	30
1	29.536
2	29.056
3	28.579
4	28.107
5	27.642
6	27.186
7	26.739
8	26.303
9	25.881
10	25.472

$$MatT := \text{augment}(x, Th, Td, Tw, Tm, Ty)$$

Matw =

	0	1	2	3	4	5
0	0	129.021	129.021	129.021	129.021	129.021
1	0.01	42.919	42.965	52.391	83.109	119.668
2	0.02	42.919	42.919	43.439	53.288	106.561
3	0.03	42.919	42.919	42.929	45.732	90.833
4	0.04	42.919	42.919	42.919	43.569	75.747
5	0.05	42.919	42.919	42.919	43.035	64.901
6	0.06	42.919	42.919	42.919	42.934	57.823
7	0.07	42.919	42.919	42.919	42.921	53.197
8	0.08	42.919	42.919	42.919	42.919	50.025
9	0.09	42.919	42.919	42.919	42.919	47.832
10	0.1	42.919	42.919	42.919	42.919	46.281

MatT =

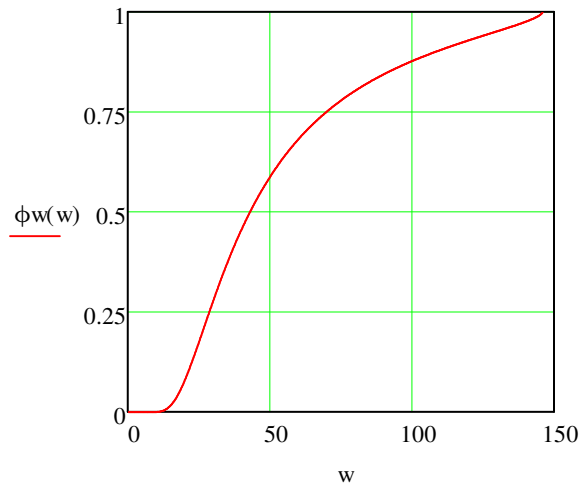
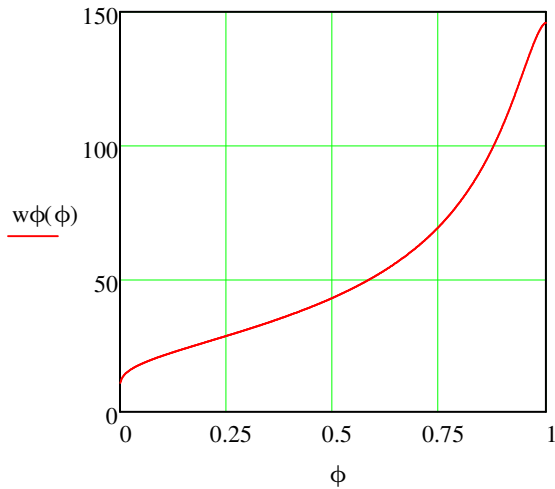
	0	1	2	3	4	5
0	0	30	30	30	30	30
1	0.5	20.001	22.494	26.641	28.348	29.536
2	1	20.001	20.212	23.84	26.749	29.056
3	1.5	20.001	20.007	21.914	25.286	28.579
4	2	20.001	20.001	20.815	24.005	28.107
5	2.5	20.001	20.001	20.295	22.931	27.642
6	3	20.001	20.001	20.09	22.069	27.186
7	3.5	20.001	20.001	20.024	21.408	26.739
8	4	20.001	20.001	20.006	20.924	26.303
9	4.5	20.001	20.001	20.002	20.583	25.881
10	5	20.001	20.001	20.001	20.354	25.472

Tref := 20      TKref := 273.15 + Tref      ρw := 1000       $\frac{R}{Mw} := 8.314$       Mw := 0.018

Sorption isotherm.

$$w\phi(\phi) := \frac{146}{\left[1 + \left(-8 \cdot 10^{-8} \cdot \frac{R \cdot TKref \cdot \rho w}{Mw} \cdot \ln(\phi)\right)^{1.6}\right]^{0.375}}$$

$$\phi w(w) := e^{\frac{-Mw}{R \cdot TKref \cdot \rho w} \cdot 0.125 \cdot 10^8 \cdot \left[\left(\frac{146}{w}\right)^{\frac{1}{0.375}} - 1\right]^{0.625}}$$



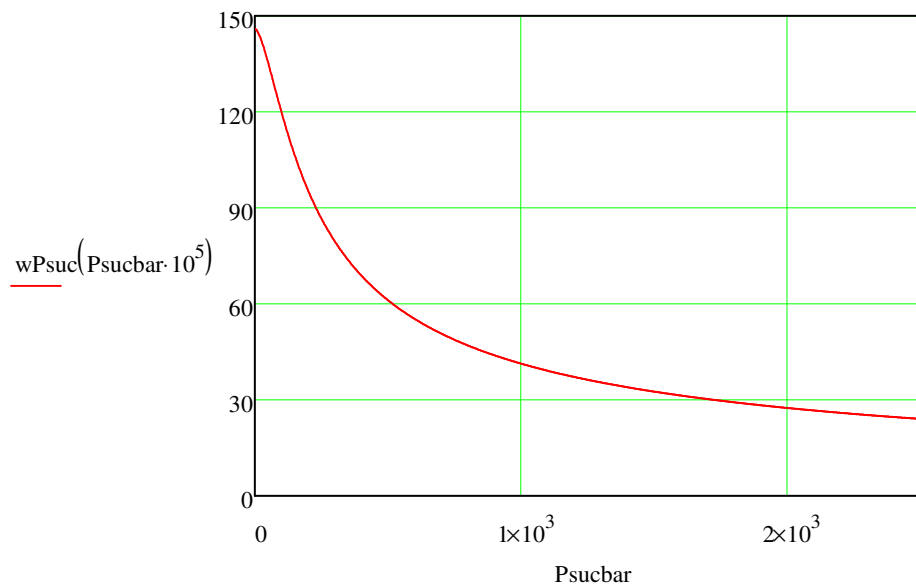
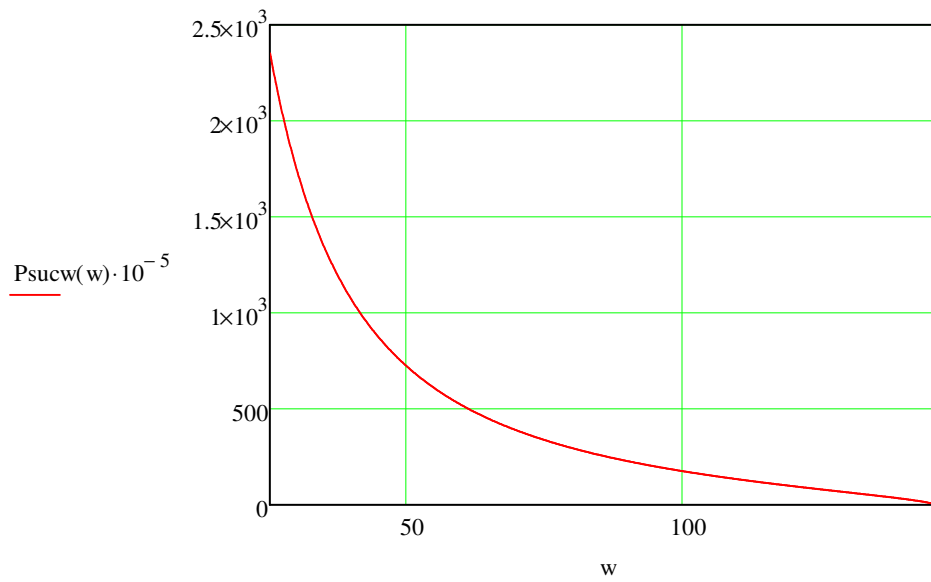
$w\phi(10^{-10}) = 5.323$  ( !! )       $w\phi(0.01) = 13.972$        $w\phi(0.5) = 42.922$        $\phi w(42.922) = 0.5$

$w\phi(0.95) = 129.021$

Water retention curve.

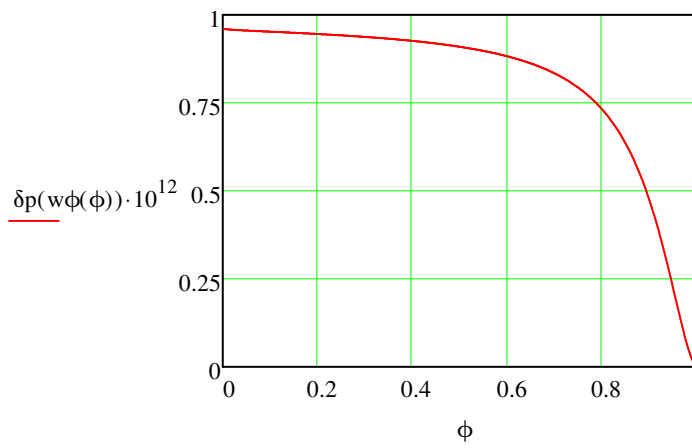
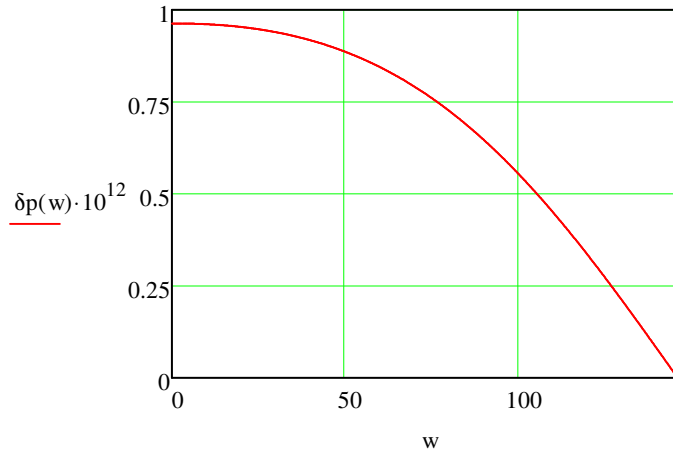
$$wPsuc(Psuc) := \frac{146}{\left[1 + \left(8 \cdot 10^{-8} \cdot Psuc\right)^{1.6}\right]^{0.375}}$$

$$Psucw(w) := 0.125 \cdot 10^8 \cdot \left[\left(\frac{146}{w}\right)^{\frac{1}{0.375}} - 1\right]^{0.625}$$



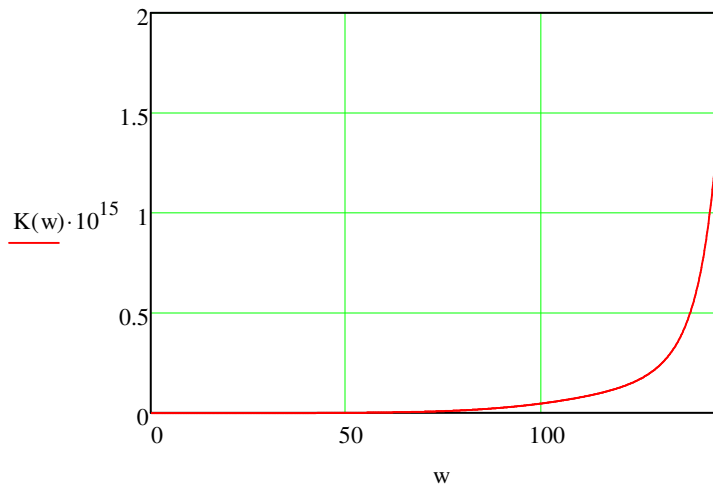
Vapor diffusion.

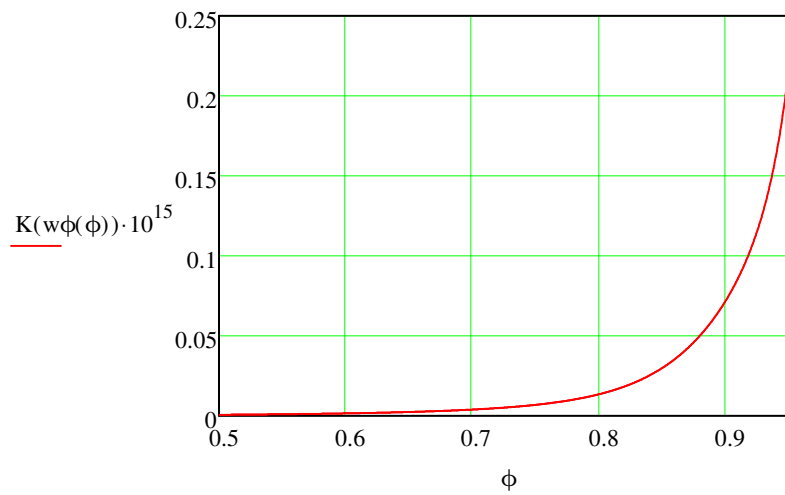
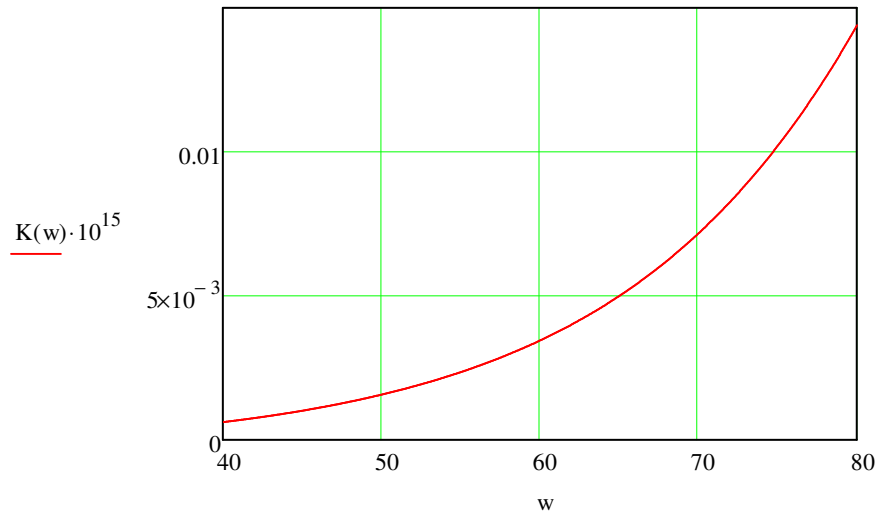
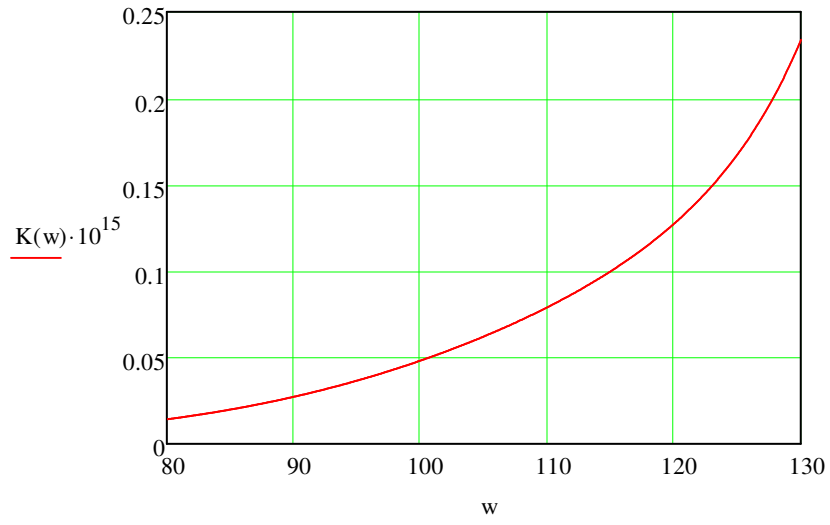
$$\delta p(w) := \frac{Mw}{R \cdot TKref} \cdot \frac{26.1 \cdot 10^{-6}}{200} \cdot \frac{1 - \frac{w}{146}}{0.503 \cdot \left(1 - \frac{w}{146}\right)^2 + 0.497}$$



Liquid water permeability.

$$K(w) := e^{-39.2619 + 0.0704 \cdot (w-73) - 1.742 \cdot 10^{-4} \cdot (w-73)^2 - 2.7953 \cdot 10^{-6} \cdot (w-73)^3 - 1.1566 \cdot 10^{-7} \cdot (w-73)^4 + 2.5969 \cdot 10^{-9} \cdot (w-73)^5}$$





### Formula for p.sat(T).

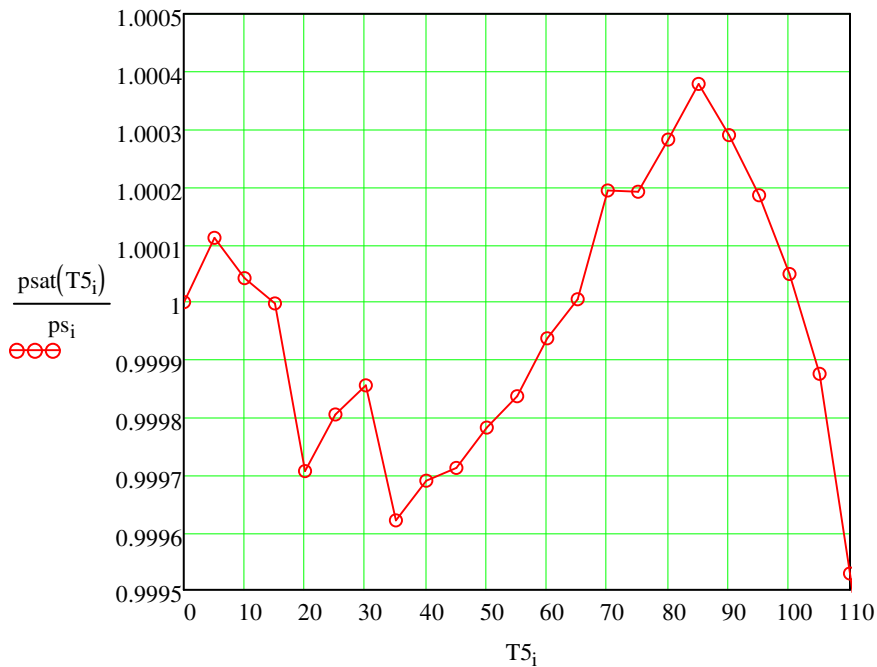
Input from table:

$$T_{ps} := \begin{pmatrix} 0 & 5 & 10 & 15 & 20 & 25 & 30 & 35 & 40 & 45 & 50 & 55 & 60 \\ 610.8 & 871.8 & 1227.0 & 1703.9 & 2337 & 3166 & 4241 & 5622 & 7375 & 9582 & 12335 & 15741 & 19920 \\ 65 & 70 & 75 & 80 & 85 & 90 & 95 & 100 & 105 & 110 & 115 & 120 & 125 \\ 25010 & 31160 & 38550 & 47360 & 57800 & 70110 & 84530 & 101330 & 120800 & 143270 & 169060 & 198540 & 232100 \end{pmatrix}$$

$$i := 0..12 \quad T5_i := T_{ps}(0,i) \quad ps_i := T_{ps}(1,i) \quad T5_{i+13} := T_{ps}(2,i) \quad ps_{i+13} := T_{ps}(3,i)$$

$$i := 0..25$$

$$Epsat(T) := \frac{19.625 \cdot T}{270.1 + T} - \frac{0.00463 \cdot T^2}{142.15 + T} \quad psat(T) := 610.8 \cdot e^{Epsat(T)}$$



Max relative error: 0.05% for 0 < T < 110.



**Boltzmann solution of coupled nonlinear equations for moisture content w(s) and temperature T(s), s=x/root(4t). Benchmark test I, CEN. New version 2012. Control and accuracy of the solution**

J. Claesson

**Input data.**

Initial and boundary conditions

$$\phi_{in} := 0.5 \quad T_{in} := 20 \quad \phi_b := 0.95 \quad T_b := 30$$

Constants

$$T_{ref} := 20 \quad T_{Kref} := 273.15 + T_{ref} \quad \rho_w := 1000 \quad R := 8.314 \quad M_w := 0.018$$

Sorption isotherm.

$$w\phi(\phi) := \frac{146}{\left[1 + \left(-8 \cdot 10^{-8} \cdot \frac{R \cdot T_{Kref} \cdot \rho_w}{M_w} \cdot \ln(\phi)\right)^{1.6}\right]^{0.375}} \quad \phi_w(w) := e^{\frac{-M_w}{R \cdot T_{Kref} \cdot \rho_w} \cdot 0.125 \cdot 10^8 \cdot \left[\left(\frac{146}{w}\right)^{0.375} - 1\right]^{0.625}}$$

Initial and boundary moisture content:

$$w_{in} := w\phi(\phi_{in}) \quad w_b := w\phi(\phi_b) \quad w_{in} = 42.922 \quad w_b = 129.021$$

Water retention curve.

$$wP_{suc}(P_{suc}) := \frac{146}{\left[1 + \left(8 \cdot 10^{-8} \cdot P_{suc}\right)^{1.6}\right]^{0.375}} \quad P_{suc}w(w) := 0.125 \cdot 10^8 \cdot \left[\left(\frac{146}{w}\right)^{0.375} - 1\right]^{0.625}$$

Vapor diffusion coefficient.

$$\delta p(w) := \frac{M_w}{R \cdot T_{Kref}} \cdot \frac{26.1 \cdot 10^{-6}}{200} \cdot \frac{1 - \frac{w}{146}}{0.503 \cdot \left(1 - \frac{w}{146}\right)^2 + 0.497}$$

Liquid water permeability.

$$K(w) := e^{-39.2619 + 0.0704 \cdot (w-73) - 1.742 \cdot 10^{-4} \cdot (w-73)^2 - 2.7953 \cdot 10^{-6} \cdot (w-73)^3 - 1.1566 \cdot 10^{-7} \cdot (w-73)^4 + 2.5969 \cdot 10^{-9} \cdot (w-73)^5}$$

Formula for p.sat(T).

$$E_{psat}(T) := \frac{19.625 \cdot T}{270.1 + T} - \frac{0.00463 \cdot T^2}{142.15 + T} \quad p_{sat}(T) := 610.8 \cdot e^{E_{psat}(T)}$$

Heat of evaporation.

$$Lev(T) := 10^6 \cdot \left[2.5016 - \frac{T}{422} - \left(\frac{T}{342}\right)^4\right]$$

Heat content (enthalpy) of water and water vapor.

$$hl(T) := 4184 \cdot T \quad hv(T) := hl(T) + Lev(T)$$

Thermal conductivity.

$$\lambda(w) := 1.5 + 0.0158 \cdot w$$

Water vapor content

$$V_p := 0.146 \quad (\text{pore volume}) \quad w_{\text{vap}}(w, T) := \left( V_p - \frac{w}{\rho_w} \right) \cdot \phi_w(w) \cdot \frac{M_w \cdot p_{\text{sat}}(T)}{R \cdot (273.15 + T)}$$

Total energy (enthalpy)

$$h(w, T) := 1.824 \cdot 10^6 \cdot T + h_l(T) \cdot w + \text{Lev}(T) \cdot w_{\text{vap}}(w, T) \quad (\text{only used for control})$$

Capacity functions (derivatives of  $h(w, T)$  ).

$$h_w(w, T) := h_l(T) + \text{Lev}(T) \cdot \frac{M_w \cdot p_{\text{sat}}(T)}{R \cdot (273.15 + T)} \cdot \left[ -\frac{\phi_w(w)}{\rho_w} + \left( V_p - \frac{w}{\rho_w} \right) \cdot \left( \frac{d}{dw} \phi_w(w) \right) \right]$$

$$h_T(w, T) := 1.824 \cdot 10^6 + 4184 \cdot w + \left( V_p - \frac{w}{\rho_w} \right) \cdot \frac{\phi_w(w) \cdot M_w}{R} \cdot \frac{d}{dT} \left( \frac{\text{Lev}(T) \cdot p_{\text{sat}}(T)}{273.15 + T} \right)$$

### Auxilliary functions.

Functions for flow coefficients:

$$K_w(w, T) := K(w) \cdot \frac{d}{dw} (-P_{\text{suc}} w(w)) + p_{\text{sat}}(T) \cdot \delta p(w) \cdot \frac{d}{dw} (\phi_w(w))$$

$$\lambda_w(w, T) := -h_l(T) \cdot K(w) \cdot \frac{d}{dw} (P_{\text{suc}} w(w)) + h_v(T) \cdot p_{\text{sat}}(T) \cdot \delta p(w) \cdot \frac{d}{dw} (\phi_w(w))$$

$$K_T(w, T) := \delta p(w) \cdot \phi_w(w) \cdot \frac{d}{dT} p_{\text{sat}}(T) \quad \lambda_T(w, T) := \lambda(w) + h_v(T) \cdot \delta p(w) \cdot \phi_w(w) \cdot \frac{d}{dT} p_{\text{sat}}(T)$$

Determinant and R-functions:

$$\text{DetK}\lambda(w, T) := K_w(w, T) \cdot \lambda_T(w, T) - K_T(w, T) \cdot \lambda_w(w, T)$$

$$R_1(w, T) := \frac{\lambda_T(w, T)}{\text{DetK}\lambda(w, T)} \quad R_2(w, T) := \frac{-K_T(w, T)}{\text{DetK}\lambda(w, T)} \quad R_3(w, T) := \frac{-\lambda_w(w, T)}{\text{DetK}\lambda(w, T)}$$

$$R_4(w, T) := \frac{K_w(w, T)}{\text{DetK}\lambda(w, T)} \quad R_5(w, T) := \frac{\lambda_T(w, T)}{\text{DetK}\lambda(w, T)} \quad R_6(w, T) := \frac{-K_T(w, T)}{\text{DetK}\lambda(w, T)}$$

$$R_7(w, T) := \frac{h_w(w, T) \cdot \lambda_T(w, T) - h_T(w, T) \cdot \lambda_w(w, T)}{\text{DetK}\lambda(w, T)} \quad R_8(w, T) := \frac{-h_w(w, T) \cdot K_T(w, T) + h_T(w, T) \cdot K_w(w, T)}{\text{DetK}\lambda(w, T)}$$

### Calculations.

Estimates of moisture and temperature penetration depths.

$$L_{\text{pen}w} := \sqrt{K_w(w_b, T_b)} \quad L_{\text{pen}T} := \sqrt{\frac{\lambda_T(w_b, T_b)}{h_T(w_b, T_b)}} \quad L_{\text{pen}w} = 8.469 \times 10^{-6} \quad L_{\text{pen}T} = 1.224 \times 10^{-3}$$

Given

$$\frac{d}{ds}w(s) = -(\mathbf{R}_1(w(s), T(s)) \cdot g(s) + \mathbf{R}_2(w(s), T(s)) \cdot q(s))$$

$$w(0) = w_b$$

$$w_b = 129.021$$

$$\frac{d}{ds}T(s) = -(\mathbf{R}_3(w(s), T(s)) \cdot g(s) + \mathbf{R}_4(w(s), T(s)) \cdot q(s))$$

$$T(0) = T_b$$

$$T_b = 30$$

$$T_{in} = 20$$

$$\frac{d}{ds}g(s) = -2 \cdot s \cdot (\mathbf{R}_5(w(s), T(s)) \cdot g(s) + \mathbf{R}_6(w(s), T(s)) \cdot q(s))$$

$$g(0) = 5.932 \cdot 10^{-4}$$

$$w_{in} = 42.922$$

$$\frac{d}{ds}q(s) = -2 \cdot s \cdot (\mathbf{R}_7(w(s), T(s)) \cdot g(s) + \mathbf{R}_8(w(s), T(s)) \cdot q(s))$$

$$q(0) = 2.369 \cdot 10^4$$

$$s_{max} := 0.003$$

$$J := 50000$$

$$\begin{pmatrix} w \\ T \\ g \\ q \end{pmatrix} := \text{Odesolve} \left[ \begin{pmatrix} w \\ T \\ g \\ q \end{pmatrix}, s, s_{max}, J \right]$$

$$i := 0..J$$

$$s_i := \frac{i}{J} \cdot s_{max}$$

$$s_{max} = 3 \times 10^{-3}$$

$$w(0) = 129.021$$

$$T(0) = 30$$

$$w(s_{max}) = 42.924$$

$$T(s_{max}) = 20.002$$

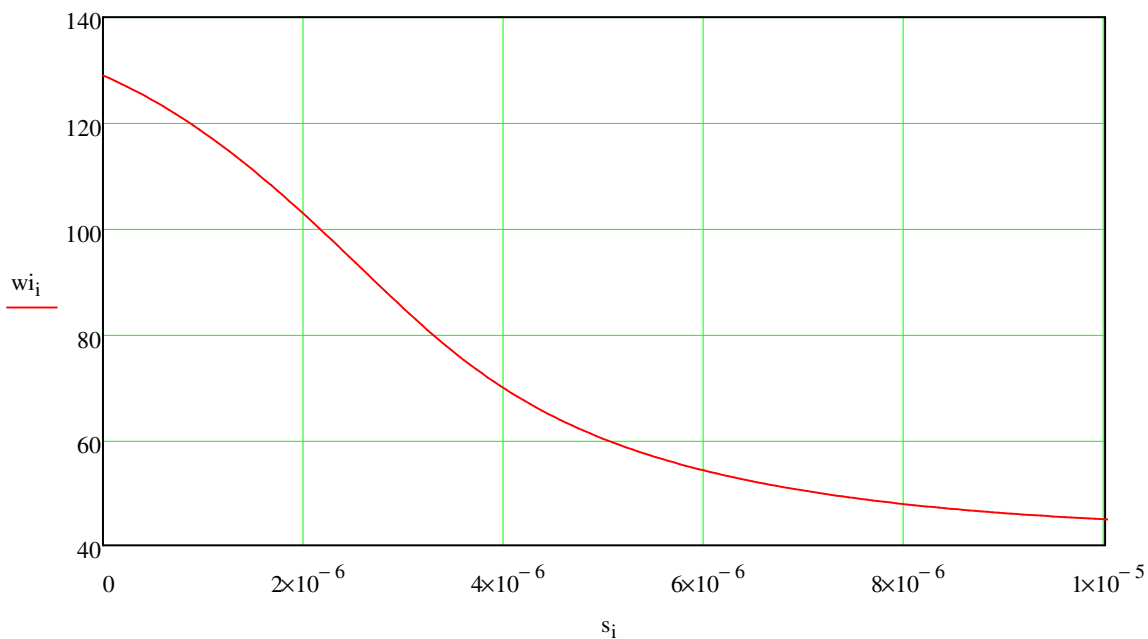
$$i := 0..J$$

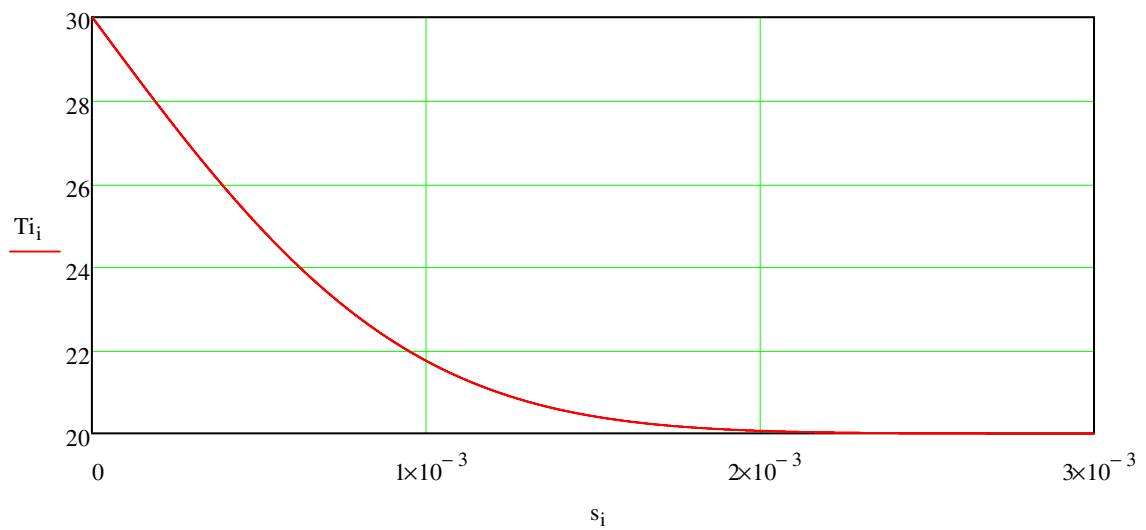
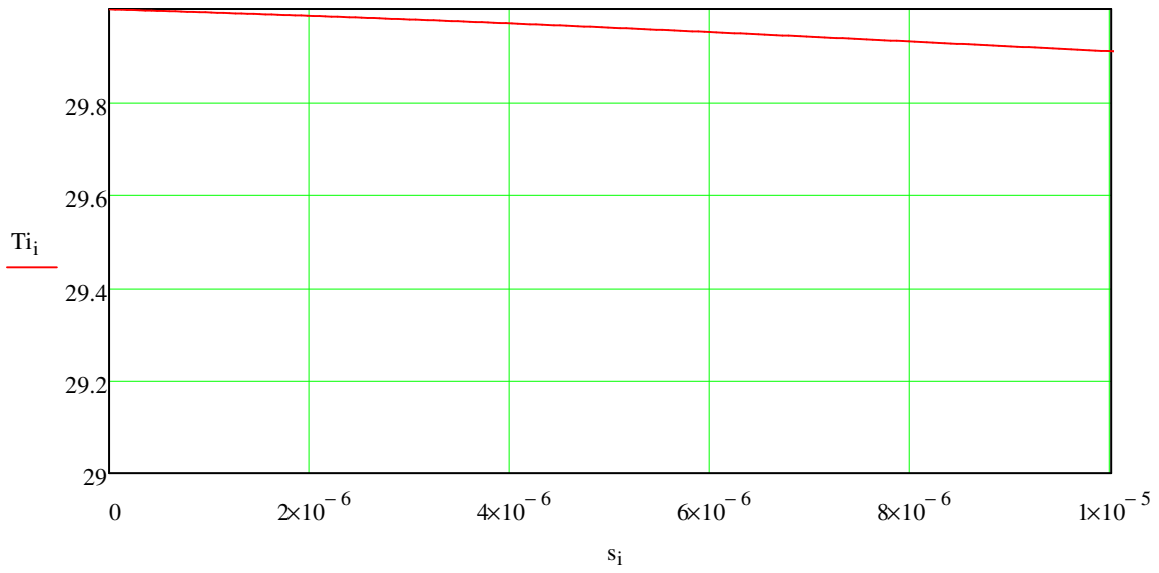
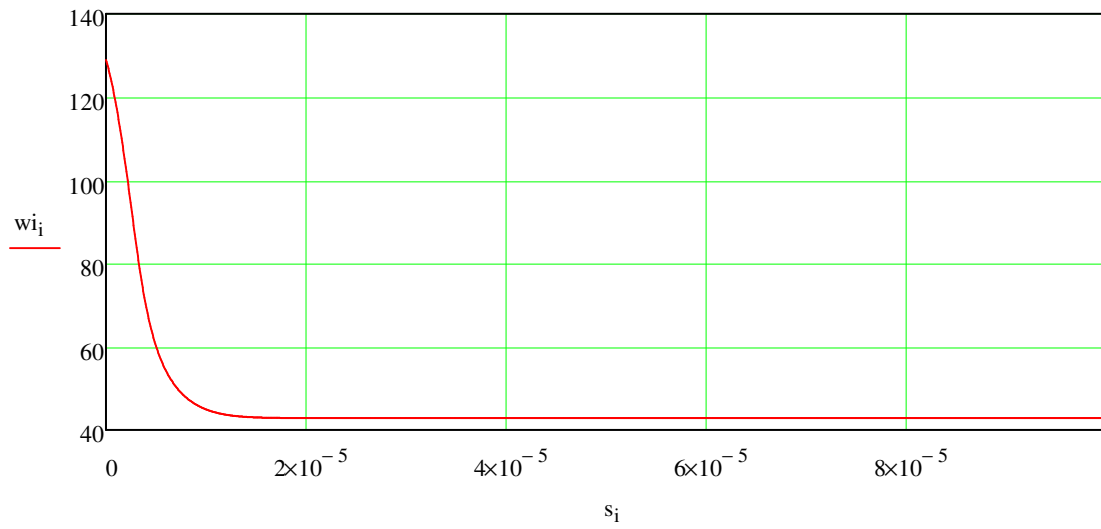
$$w_i := w(s_i)$$

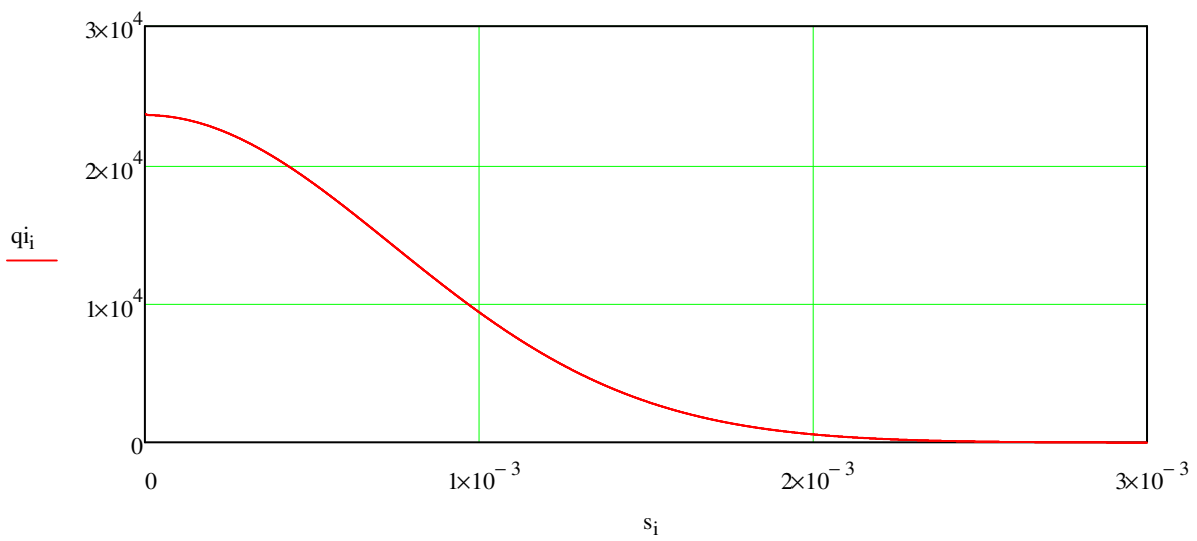
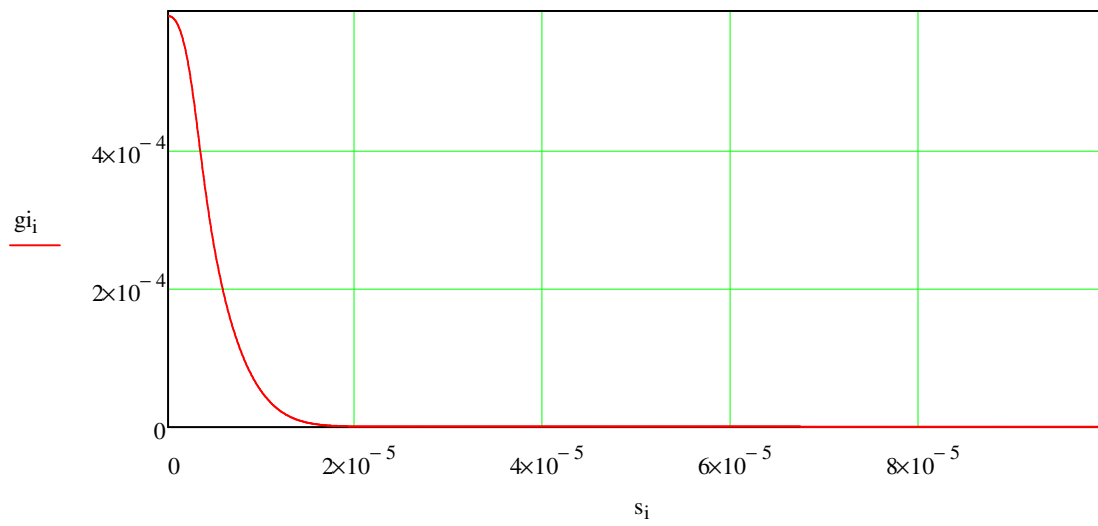
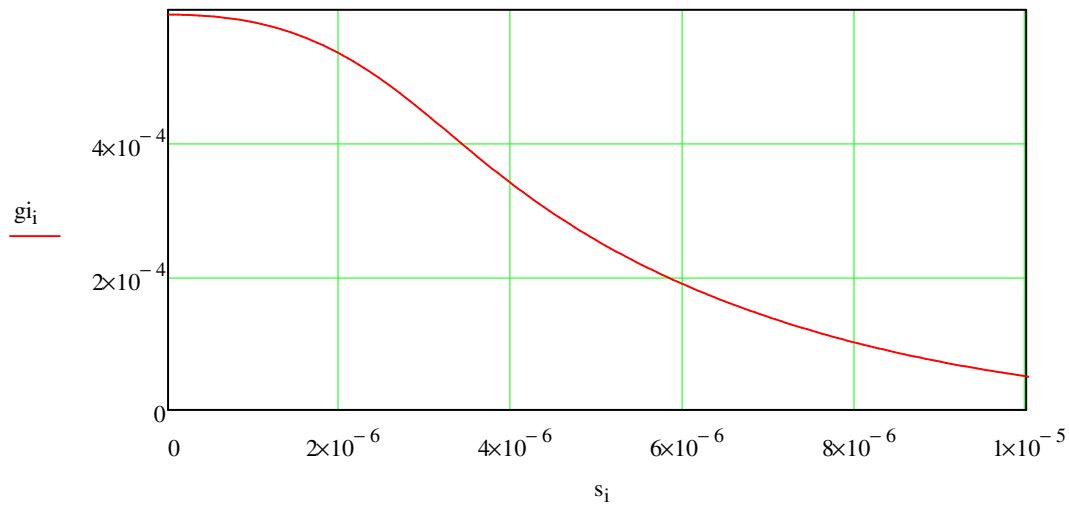
$$T_i := T(s_i)$$

$$g_i := g(s_i)$$

$$q_i := q(s_i)$$







**Control of solution.**

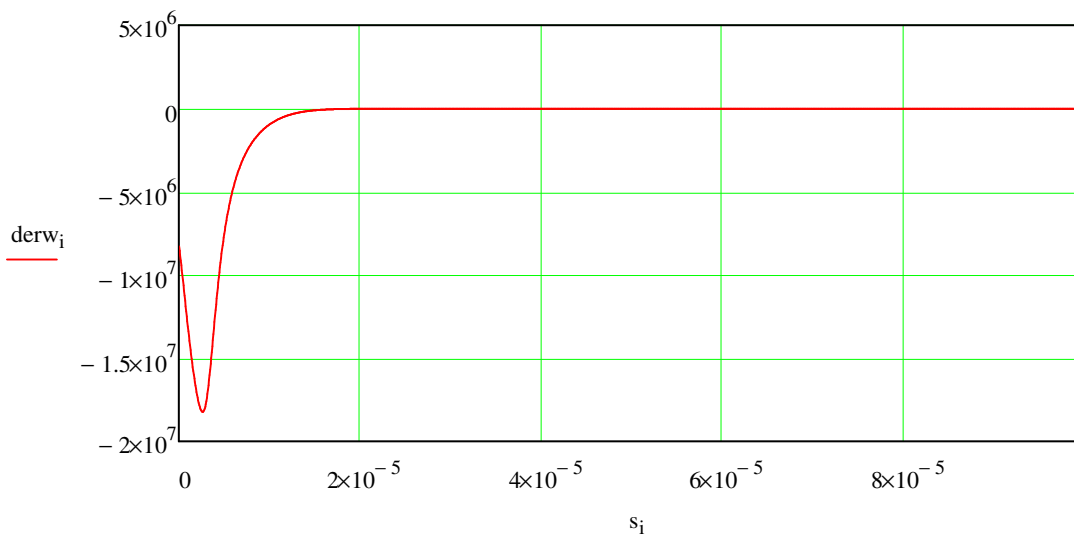
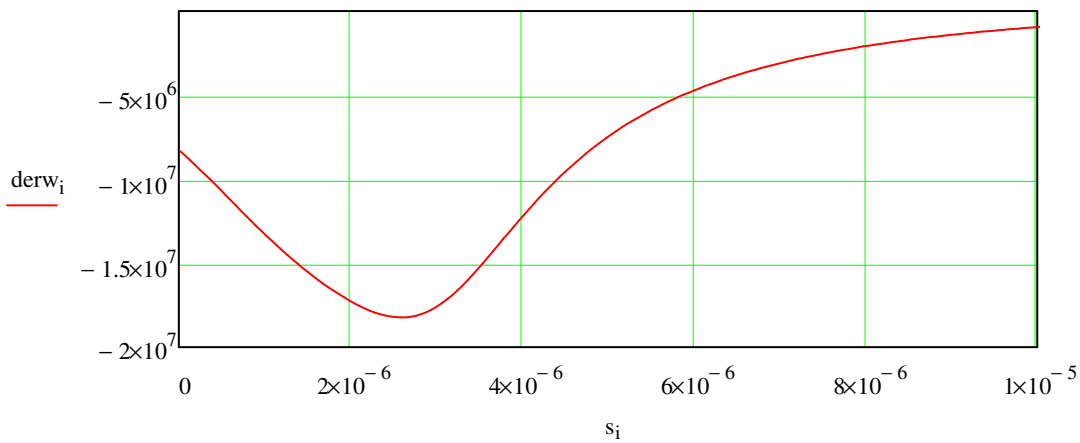
Derivatives of w, T, g and q

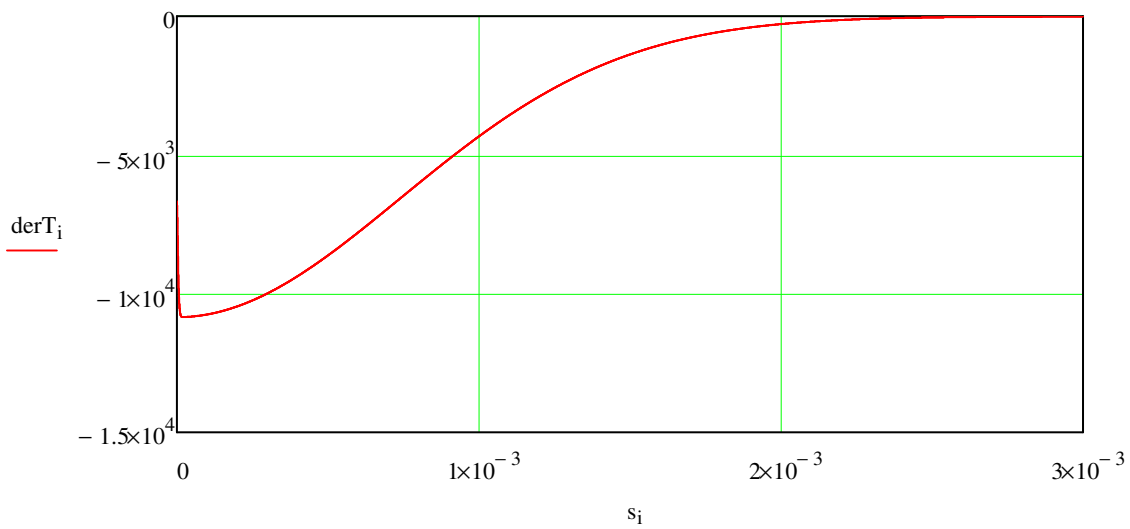
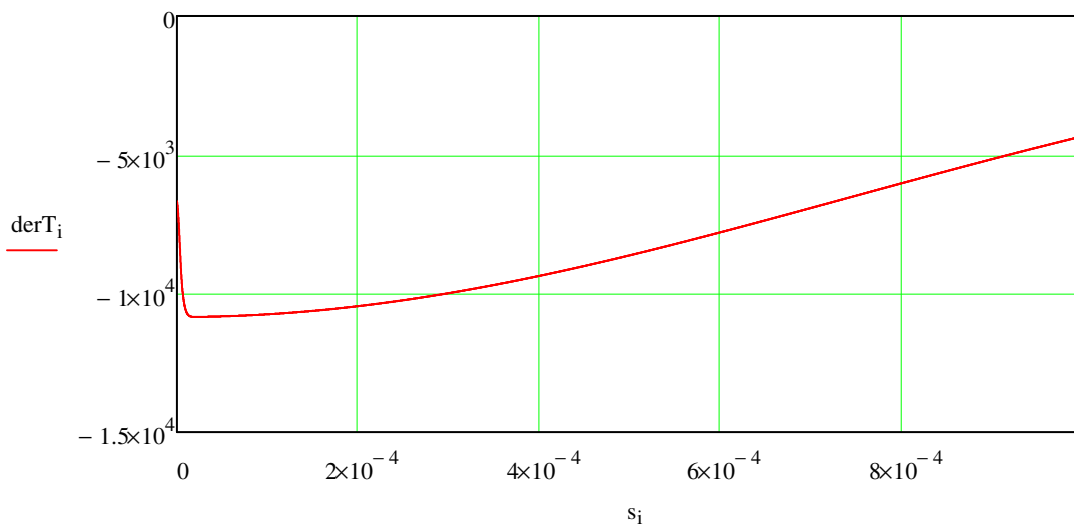
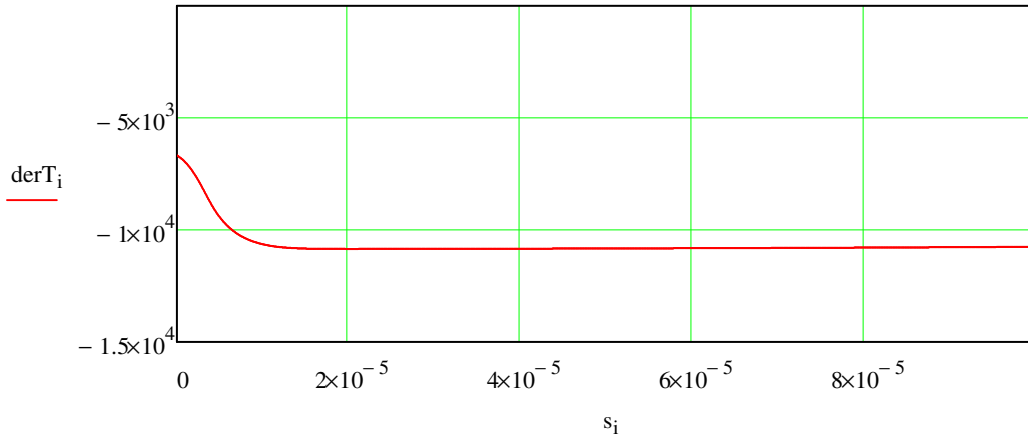
$$i := 0..J \quad \text{Det}_i := Kw(w_i, Ti_i) \cdot \lambda T(w_i, Ti_i) - KT(w_i, Ti_i) \cdot \lambda w(w_i, Ti_i)$$

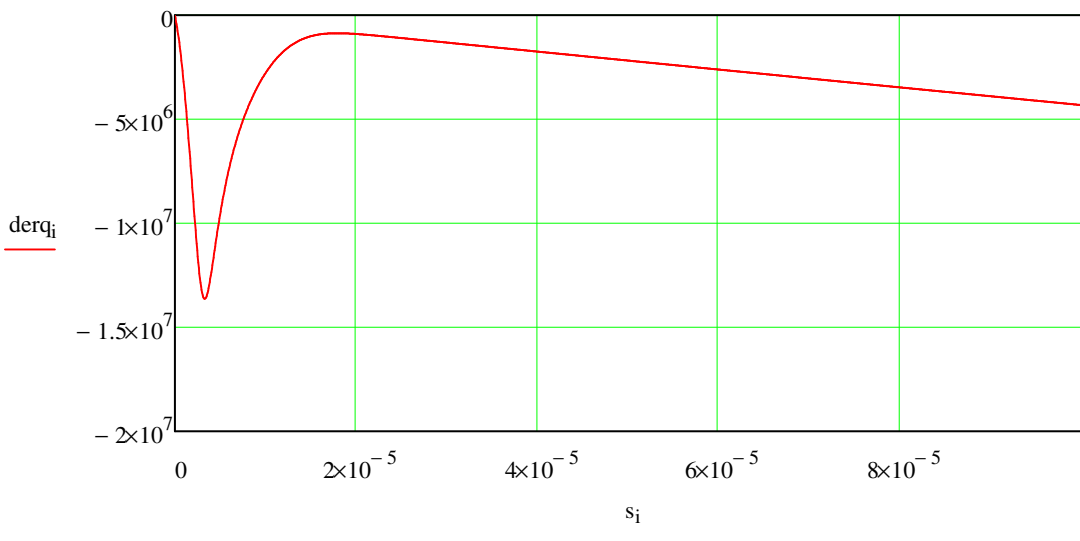
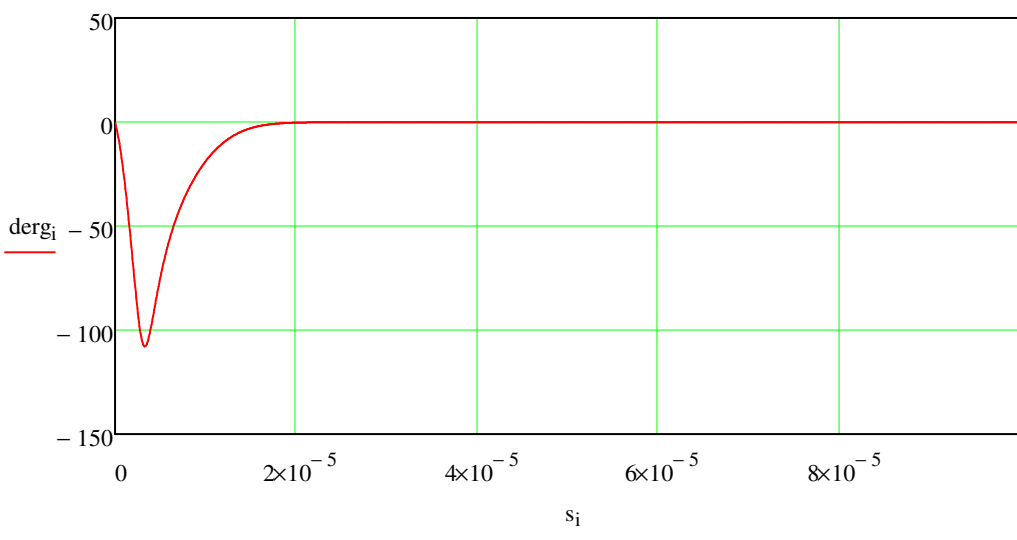
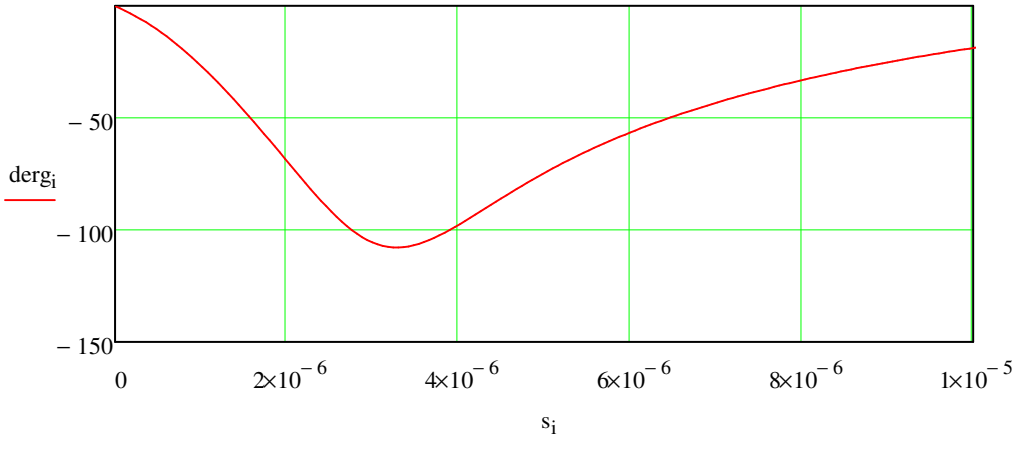
$$\text{der}w_i := -\frac{\lambda T(w_i, Ti_i) \cdot g_i - KT(w_i, Ti_i) \cdot q_i}{\text{Det}_i} \quad \text{der}T_i := -\frac{-\lambda w(w_i, Ti_i) \cdot g_i + Kw(w_i, Ti_i) \cdot q_i}{\text{Det}_i}$$

$$\text{der}g_i := -2 \cdot s_i \cdot \frac{\lambda T(w_i, Ti_i) \cdot g_i - KT(w_i, Ti_i) \cdot q_i}{\text{Det}_i} \quad R7_i := hw(w_i, Ti_i) \cdot \lambda T(w_i, Ti_i) - hT(w_i, Ti_i) \cdot \lambda w(w_i, Ti_i)$$

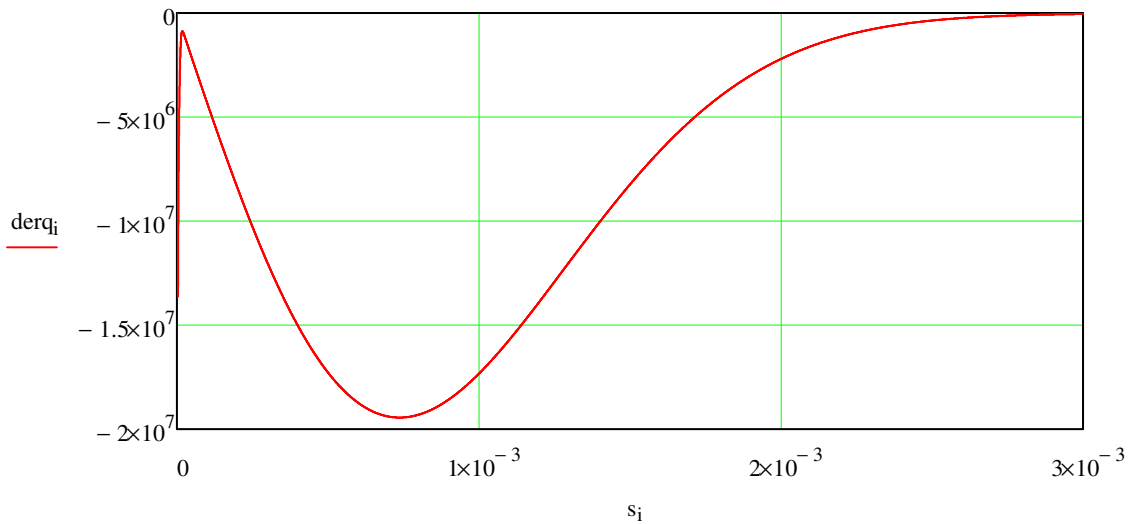
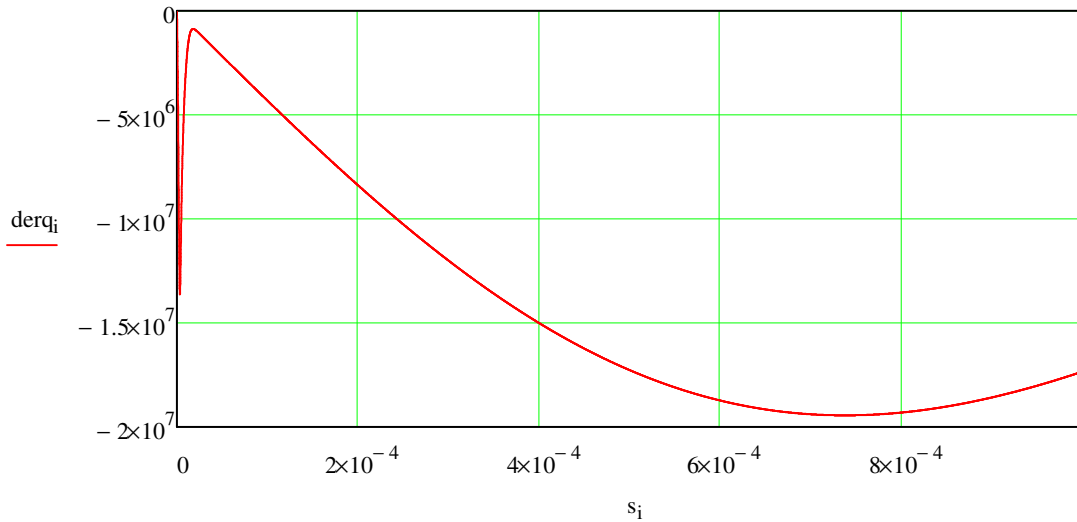
$$\text{der}q_i := -2 \cdot s_i \cdot \frac{R7_i \cdot g_i - (hw(w_i, Ti_i) \cdot KT(w_i, Ti_i) - hT(w_i, Ti_i) \cdot Kw(w_i, Ti_i)) \cdot q_i}{\text{Det}_i}$$











Errors for the four coupled ordinary differential equations:

$i := 1..J - 1$

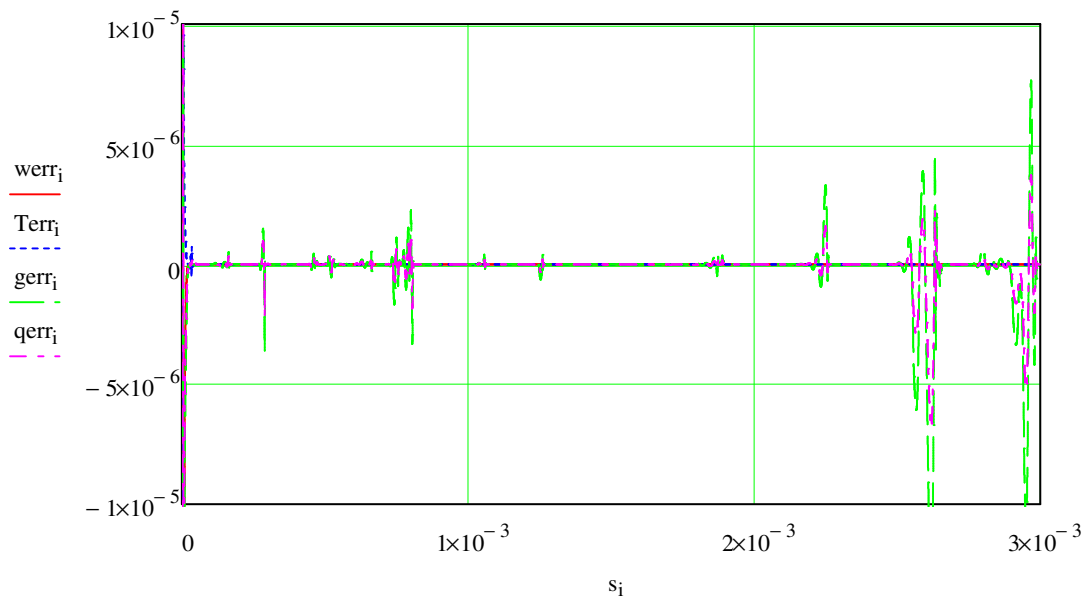
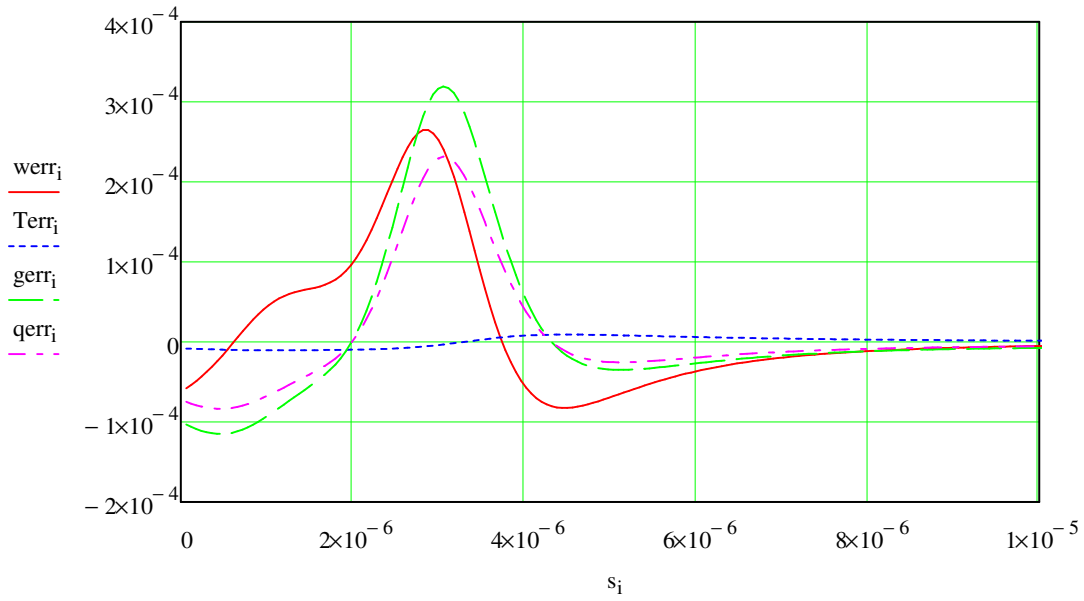
$$\text{werr}_i := \frac{\frac{w_{i+1} - w_{i-1}}{s_{i+1} - s_{i-1}} - \text{derw}_i}{1.8 \cdot 10^7}$$

$$\text{Terr}_i := \frac{\frac{T_{i+1} - T_{i-1}}{s_{i+1} - s_{i-1}} - \text{derT}_i}{11000}$$

$$\text{gerr}_i := \frac{\frac{g_{i+1} - g_{i-1}}{s_{i+1} - s_{i-1}} - \text{derg}_i}{110}$$

$$\text{qerr}_i := \frac{\frac{q_{i+1} - q_{i-1}}{s_{i+1} - s_{i-1}} - \text{derq}_i}{1.9 \cdot 10^7}$$

Note: maxima derw=1.8\*10<sup>7</sup>, derT=11000, derg=110, derq=1.9\*10<sup>7</sup>



**Conclusion: Errors below 0.03%.**

Vapor and liquid moisture flux.

$$i := 0..J$$

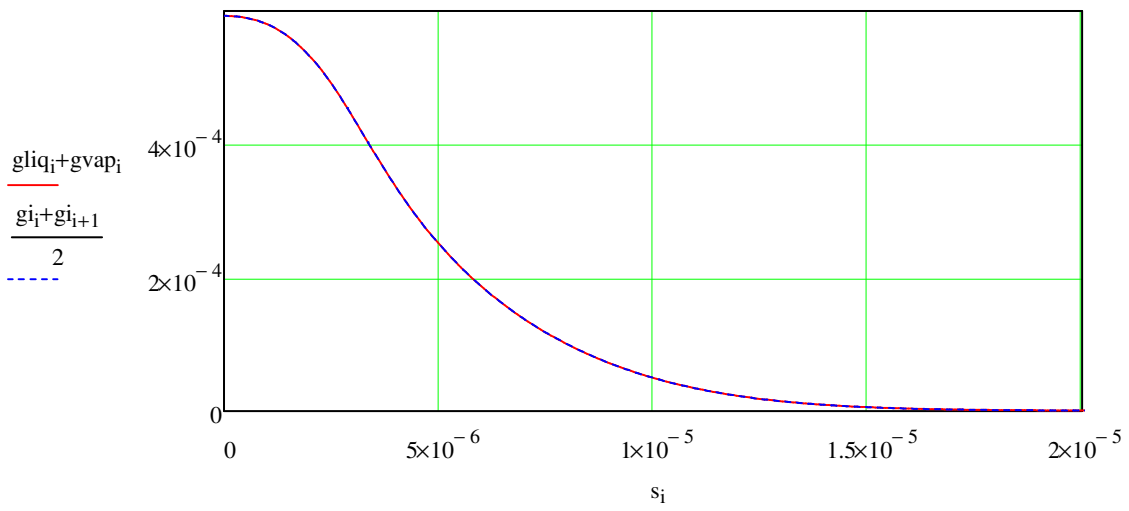
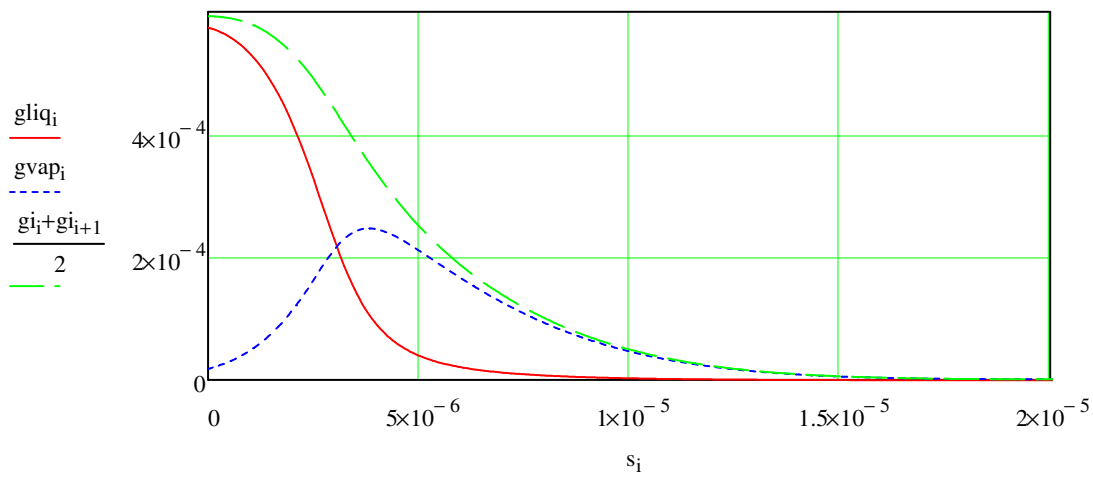
$$Psuc_i := Psucw(w_i)$$

$$p_i := \phi w(w_i) \cdot psat(T_i)$$

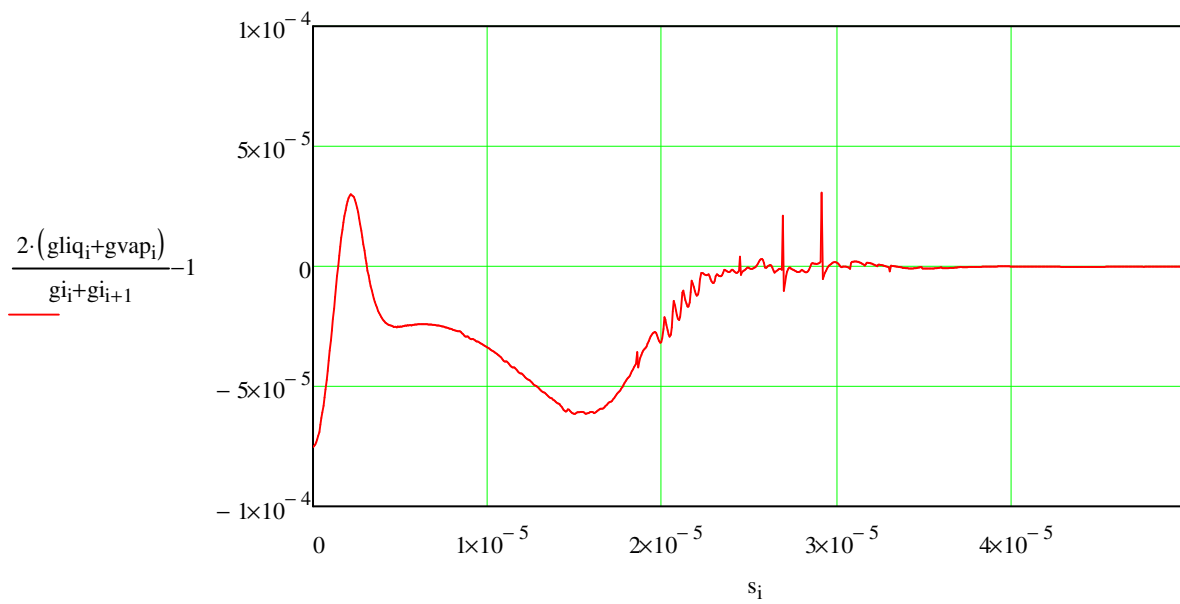
$$i := 0..J - 1$$

$$g_{liq_i} := K \left( \frac{w_i + w_{i+1}}{2} \right) \cdot \frac{Psuc_{i+1} - Psuc_i}{s_{i+1} - s_i}$$

$$g_{vap_i} := -\delta p \left( \frac{w_i + w_{i+1}}{2} \right) \cdot \frac{p_{i+1} - p_i}{s_{i+1} - s_i}$$

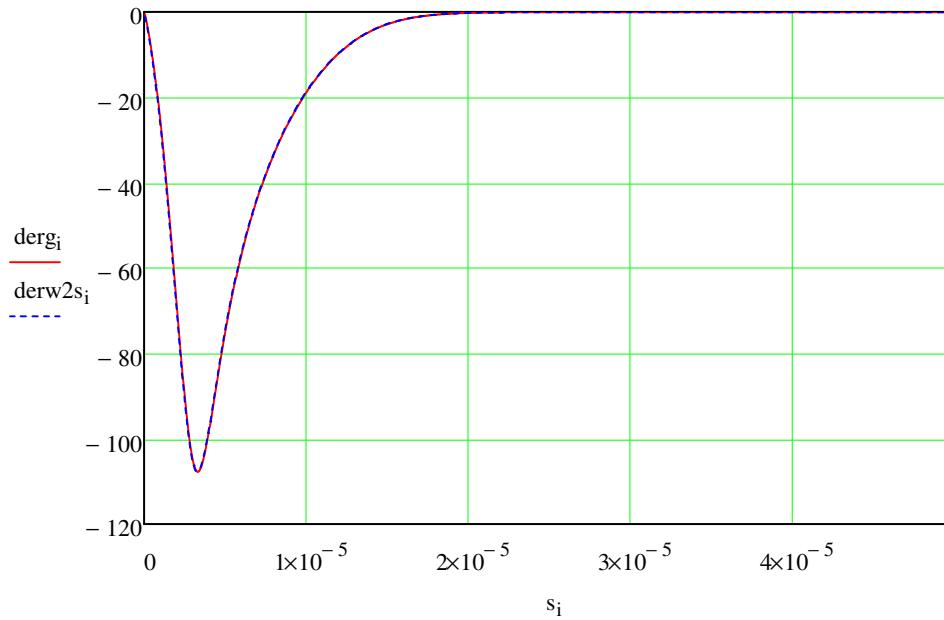


$$g_{liq_{J-1}} + g_{vap_{J-1}} = 1.812 \times 10^{-10}$$

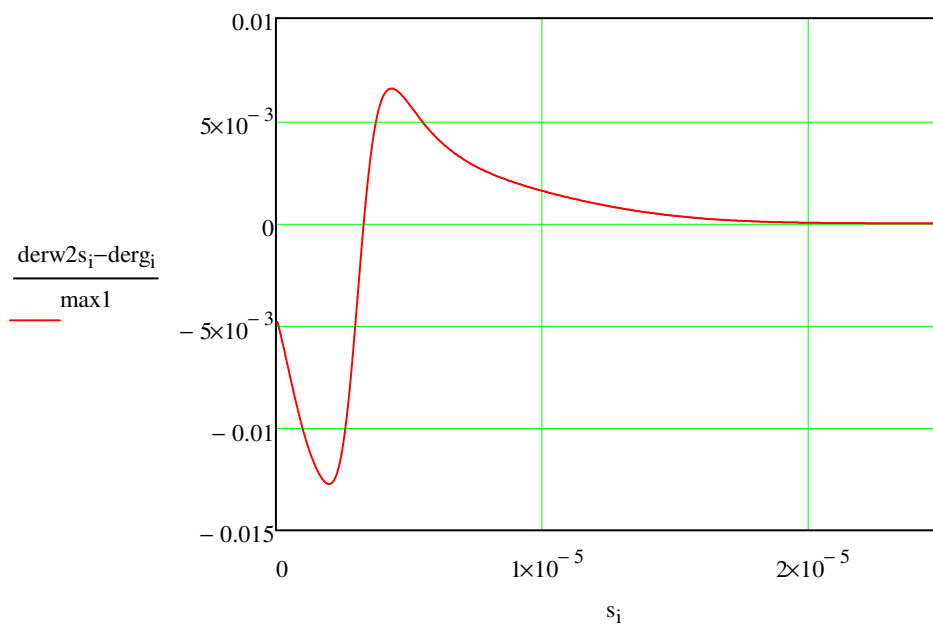


Moisture balance.

$$i := 1..J - 1 \quad \text{derg}_i := \frac{g_i - g_{i-1}}{0.5 \cdot (s_{i+1} - s_{i-1})} \quad \text{derw2s}_i := 2 \cdot s_i \cdot \frac{w_{i+1} - w_{i-1}}{s_{i+1} - s_{i-1}}$$

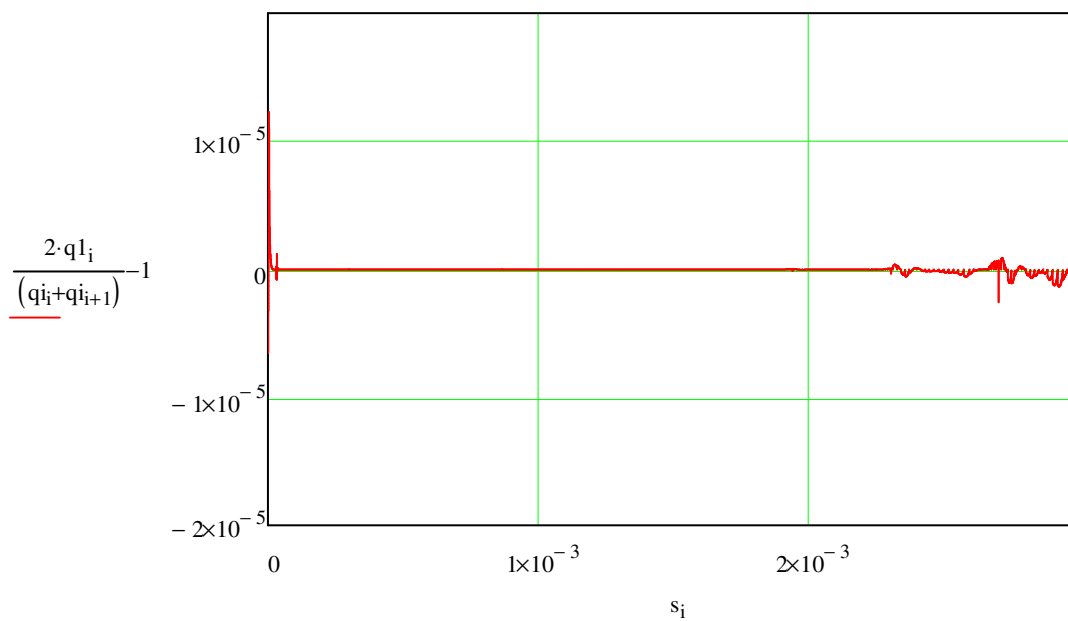
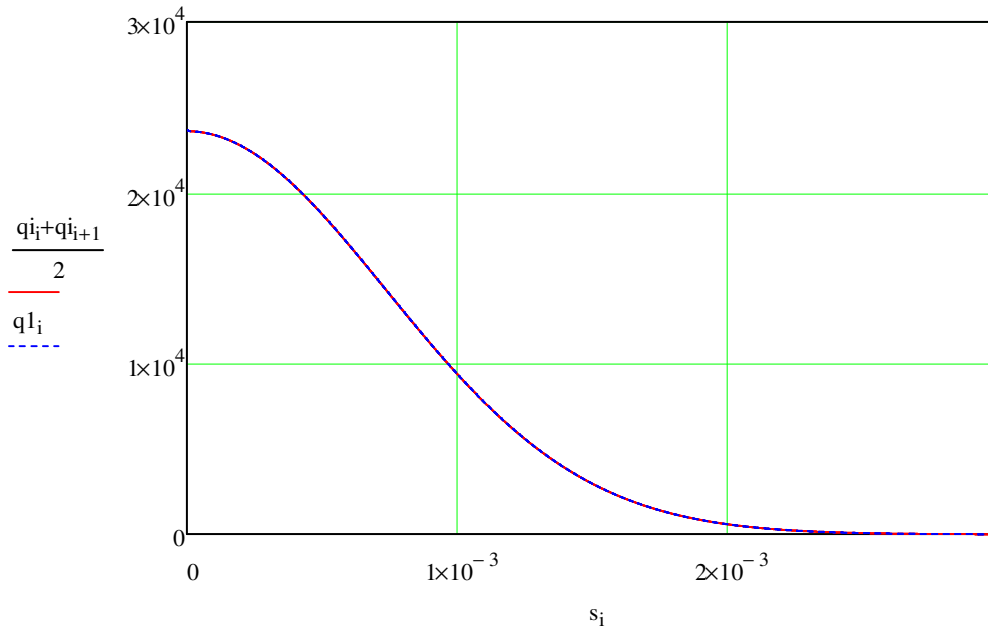


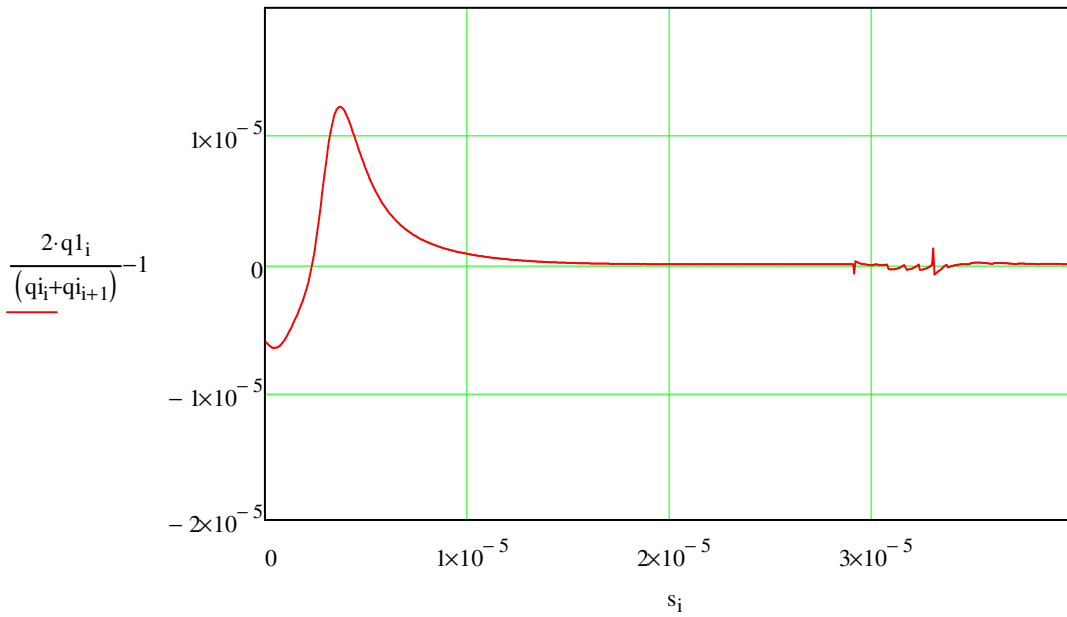
$$\text{max1} := \max(-\text{derg}) \quad \text{max1} = 107.685$$



Enthalpy flux.

$$q1_i := -\lambda \left( \frac{w_i + w_{i+1}}{2} \right) \cdot \frac{T_{i+1} - T_i}{s_{i+1} - s_i} + hl \left( \frac{T_i + T_{i+1}}{2} \right) \cdot g_{liq_i} + hv \left( \frac{T_i + T_{i+1}}{2} \right) \cdot g_{vap_i}$$



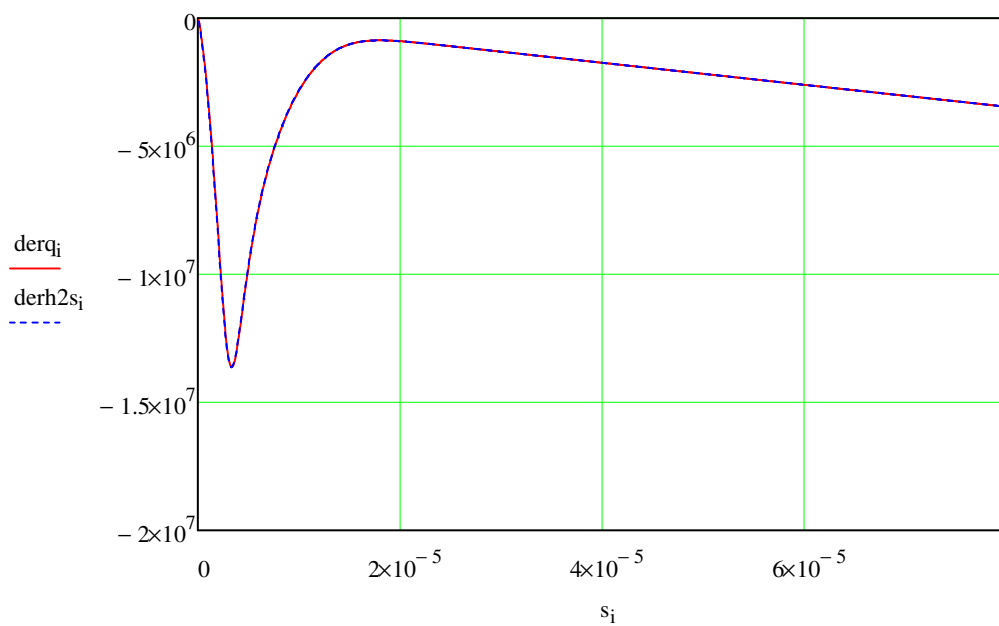


Energy (enthalpy) balance.

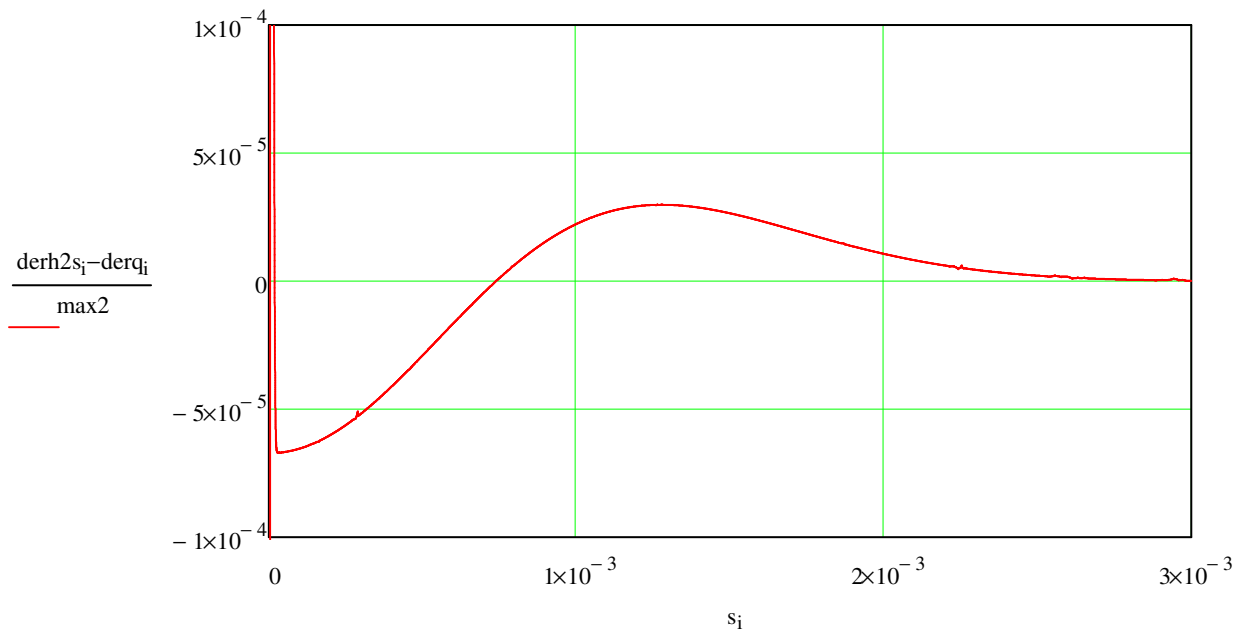
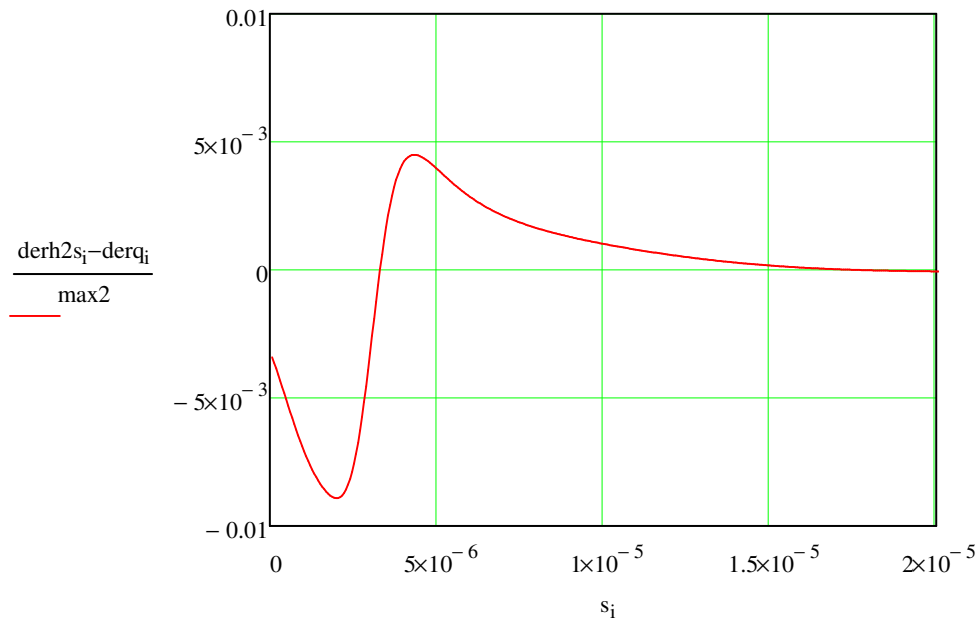
$$i := 0..J$$

$$h1_i := h(wi_i, Ti_i)$$

$$i := 1..J - 1 \quad \text{derq}_i := \frac{q_i - q_{i-1}}{0.5 \cdot (s_{i+1} - s_{i-1})} \quad \text{derh2s}_i := 2 \cdot s_i \cdot \frac{h1_{i+1} - h1_{i-1}}{s_{i+1} - s_{i-1}}$$



$$\text{max2} := \max(-\text{derq}) \quad \text{max2} = 1.943 \times 10^7$$

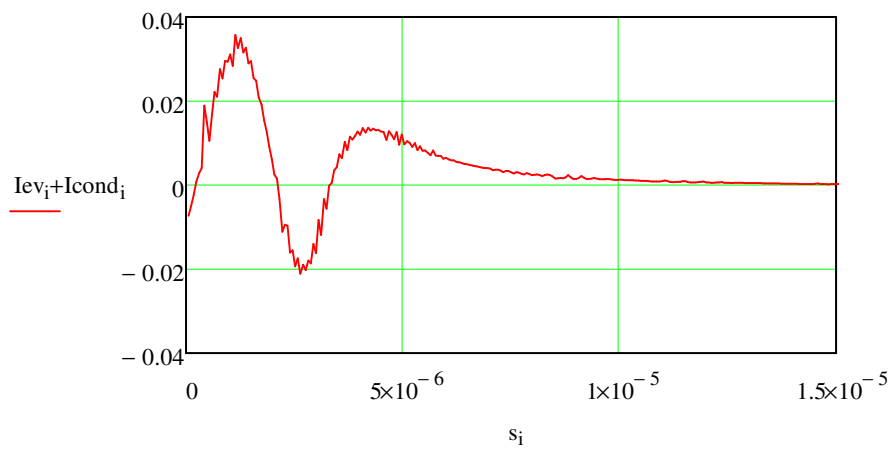
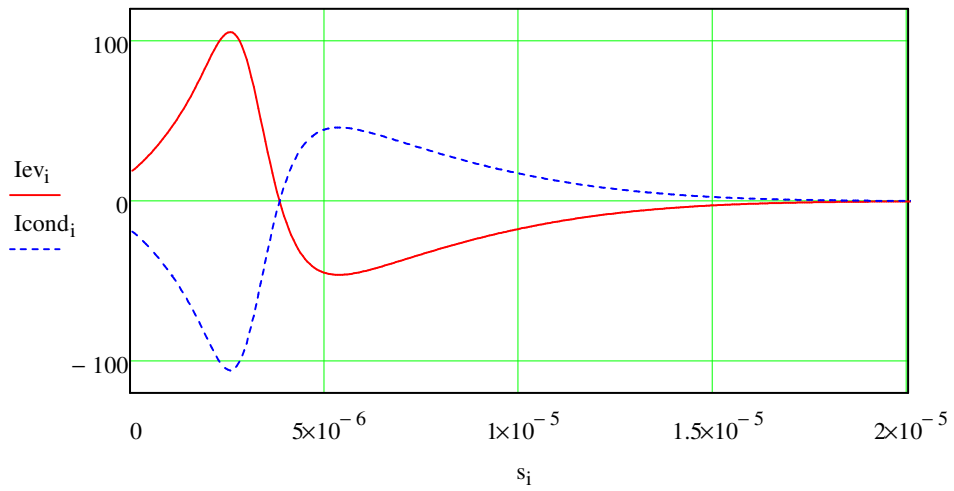


Evaporation and condensation of moisture.

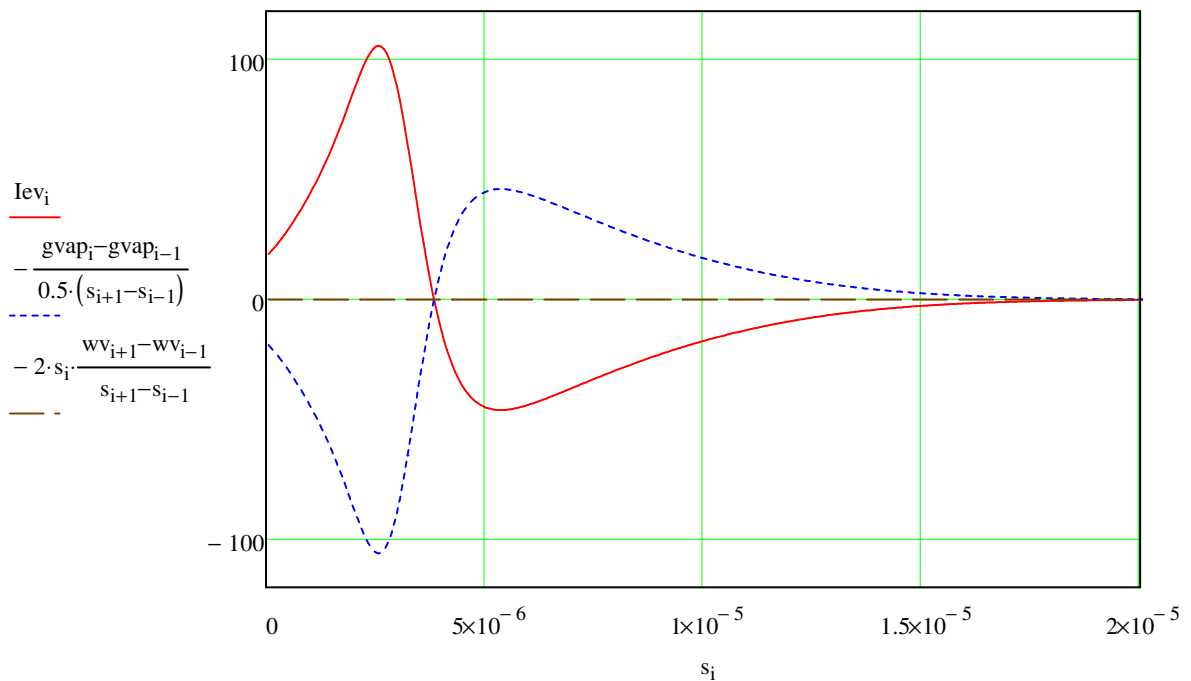
$$i := 0..J \quad wv_i := wv_{\text{vap}}(wi_i, Ti_i) \quad wl_i := wi_i - wv_i$$

$$i := 1..J - 1 \quad I_{\text{ev}}_i := -2 \cdot s_i \cdot \frac{wv_{i+1} - wv_{i-1}}{s_{i+1} - s_{i-1}} + \frac{gv_{\text{vap}_i} - gv_{\text{vap}_{i-1}}}{0.5 \cdot (s_{i+1} - s_{i-1})}$$

$$I_{\text{cond}}_i := -2 \cdot s_i \cdot \frac{wl_{i+1} - wl_{i-1}}{s_{i+1} - s_{i-1}} + \frac{g_{\text{liq}_i} - g_{\text{liq}_{i-1}}}{0.5 \cdot (s_{i+1} - s_{i-1})}$$

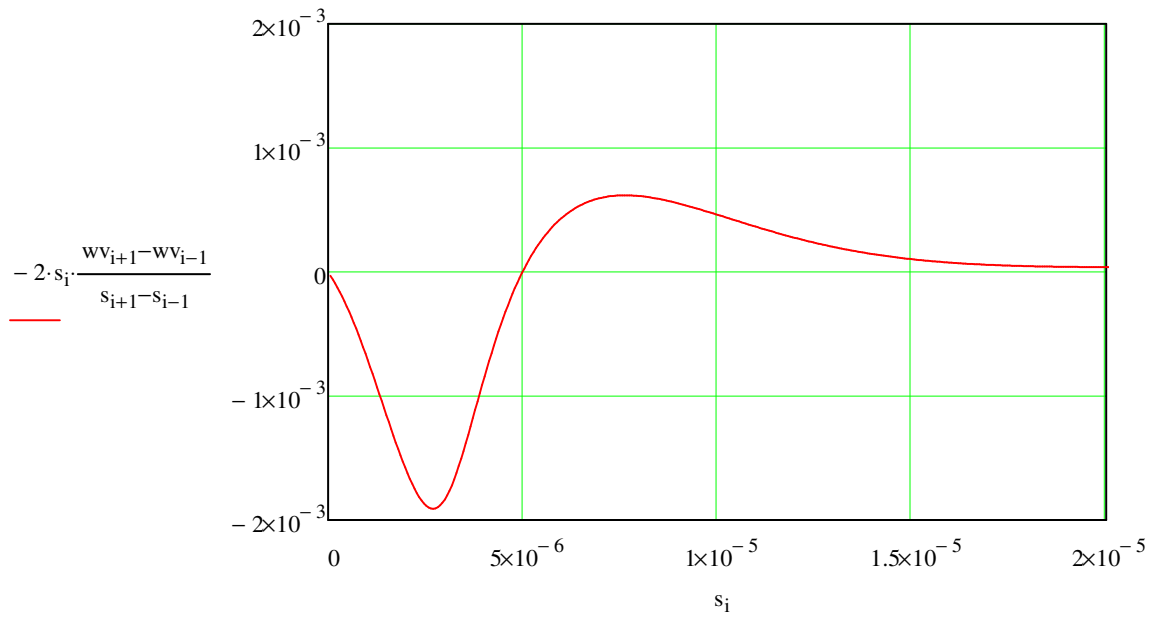


Vapor balance: Evaporation + net influx = rate of increase for water vapor content.

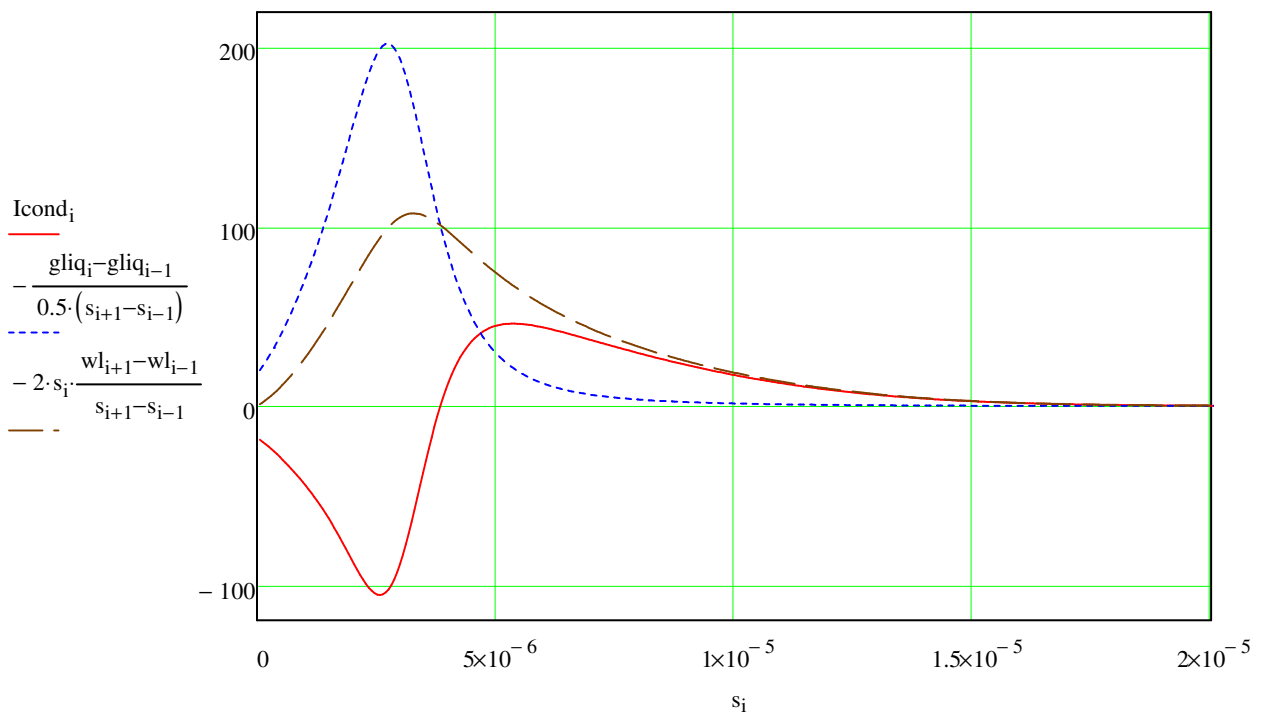




Rate of increase for water vapor content.



Balance for liquid water: Condensation + net influx = rate of increase for liquid water content.



**Curves for presentation.**

$$i := 1..J - 1$$

$$l_{liqconv,i} := -\frac{g_{liq,i} - g_{liq,i-1}}{0.5 \cdot (s_{i+1} - s_{i-1})}$$

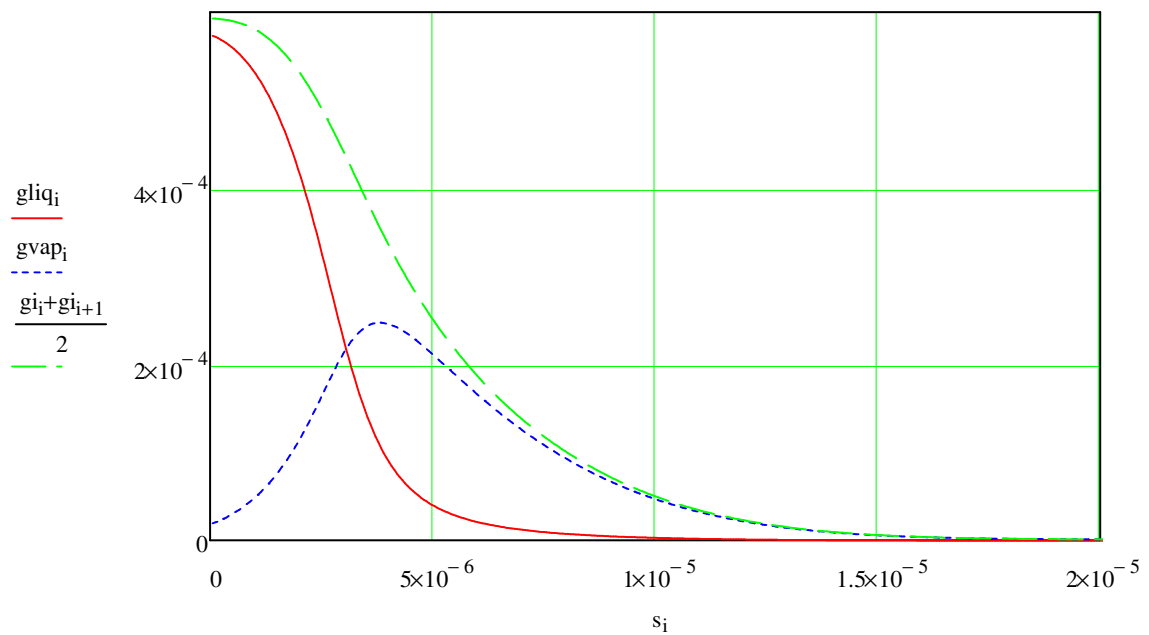
$$l_{liqinc,i} := -2 \cdot s_i \cdot \frac{w_{l,i+1} - w_{l,i-1}}{s_{i+1} - s_{i-1}}$$

$$l_{vapconv,i} := -\frac{g_{vap,i} - g_{vap,i-1}}{0.5 \cdot (s_{i+1} - s_{i-1})}$$

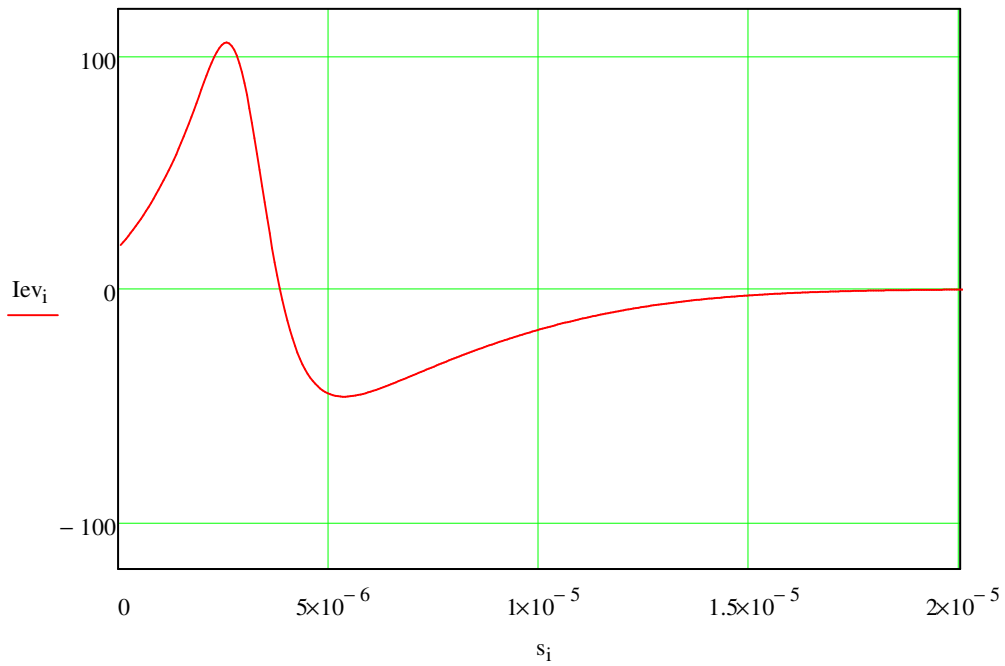
$$l_{vap,i} := -2 \cdot s_i \cdot \frac{w_{v,i+1} - w_{v,i-1}}{s_{i+1} - s_{i-1}}$$

**Liquid and vapor flux of water**

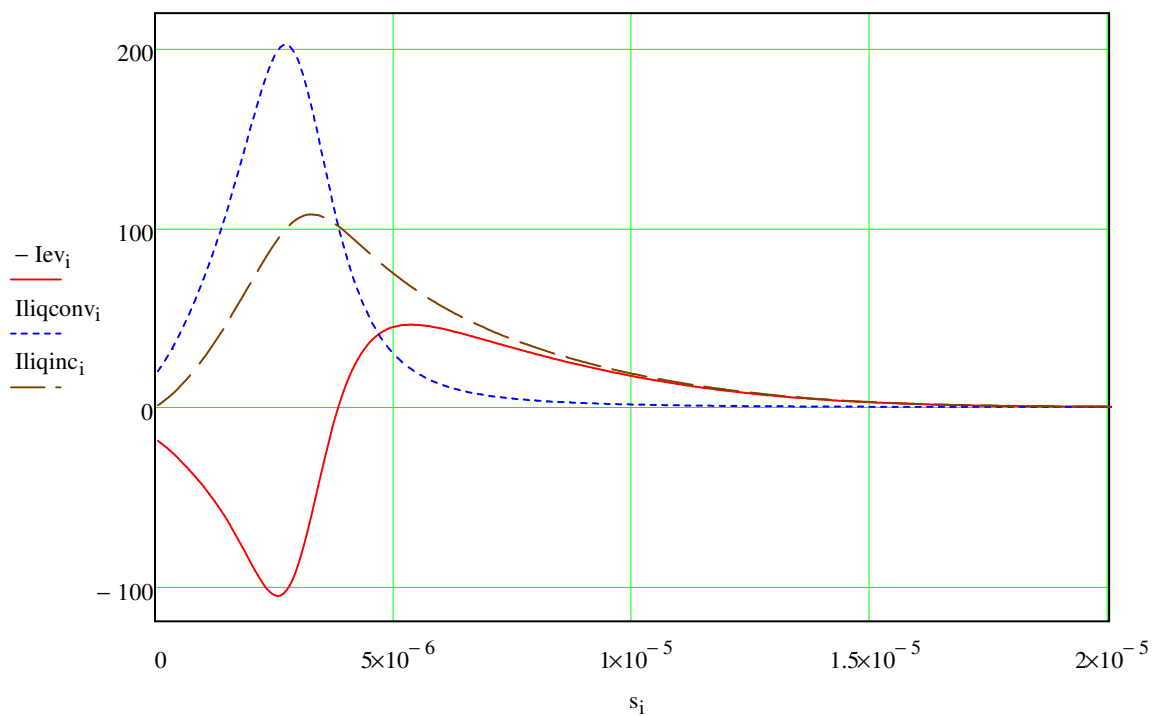
Benchmark test I, CEN. J. Claesson



## Rate of evaporation



Balance for liquid water: Condensation (  $-I_{ev}$  ) + net influx (  $I_{liqconv}$  ) = rate of increase for liquid water content (  $I_{liqinc}$  ).



Balance for water vapor: Evaporation (  $I_{ev}$  ) + net influx (  $I_{vapconv}$  ) = rate of increase for water vapor content (  $I_{vapinc}$  ).

