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Sustainpack

Innovation and Sustainable Development in the Fibre Based Packaging Value Chain

Instrument: **IP**

D2.76: Improvement of model based optimisation of demonstrator process conditions

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PU	Public	X
PP	Restricted to other programme participants (including the Commission Services)	
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IMPROVEMENT OF MODEL BASED OPTIMISATION OF DEMONSTRATOR PROCESS CONDITIONS

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Summary

Summary	PTS carried out various trials with microfibrillated cellulose (MFC) in order to improve the bending stiffness and z-strength of a 3-layered board, critical paper properties within SP2/WP2.2 demonstrator trials. Additionally a numerical simulation model, consisting of a set of equations to be implemented in customary spread sheet applications, was developed, which helps to calculate optimal parameters for material selection and process conditions under various constraints.
Results and Recommendation	Depending on the dewatering conditions acceptable for top/back layers, the total weight of the 3-ply-board can be decreased by 2-6 % when adding MFC whilst maintaining a given level of z-strength and bending stiffness.

Content

1 Introduction

Objectives of WP 2.2

The key objective in WP2.2 is to improve the strength properties of paperboard by 30% in order to reduce the material consumption. The goal of the demonstrator project is to compare a number of technologies which have been devised to reduce the material need in a three layer board construction whilst maintaining bending stiffness and z-strength.

One new and innovative technology is the use of nanomaterials to improve paper properties.

MFC trials at PTS

Different trials with microfibrillated celluloses (MFC) carried out at PTS were reported in deliverable D2.72 [1]. STFI supplied MFC 004005/001 (furthermore called MFC-1). Three different pulps (CTMP, softwood and hardwood chemical pulps) were used under various refining conditions. It was reported that a weight reduction of up to 5% is possible in the middle layer.

In contrast to D2.72 the focus of D2.76 was on adding MFC 004007/009 (supplied by STFI, furthermore called MFC-2) to a pulp composition used in the top-layer in order to increase the stiffness. In addition to this, the dosage strategy was adapted to the conditions prevailing in the approach flow system of a paper machine.

Model based optimisation

In deliverable D2.71 [8] PTS developed a numerical simulation model which helps to optimize the selection of materials and process conditions (fractionating, refining, blending). After the recent trials with MFC-2 a critical mass of experimental data is available which can be used to improve the simulation model in such a way that the influences of MFC quality and addition can be considered and can be combined with the various other technologies.

Used abbreviations (in alphabetical order)

Abbreviation/Symbol	**Meaning**
ρ_W	Cellulose density [~ 1,48 g/cm^3)
A_B	Bonded fibre area per elementary cell [µm^2]
A_{CSA}	Fibre cross section area (collapsed/dried) [µm^2]
AD	Apparent density [g/cm^3]
A_T	Total fibre area per elementary cell [µm^2]
b	Bonding strength [MPa]
BS	Bending stiffness [mNm]
CWT	Cell wall thickness [µm]
D	Fibre diameter (collapsed/dried) [µm]
d	Distance in the reference fibre network
EM	Elastic modulus [MPa]
FL	Fibre length [mm]
H	Fibre height (collapsed/dried) [µm]
K	Specific light absorption coefficient [m^2/kg]
P	Fibre perimeter (collapsed/dried) [µm]
PEI	Polymin SK as retention agent
RBA	Relative bonded area
s	Specific light scattering coefficient [m^2/kg]
SB	Scott-Bond [J/m^2]
SEL	Specific edge load [Ws/m]
SR	SCHOPPER-RIEGLER value [°]
SRE	Specific refining energy [kWh/t]
SSA	Specific surface area [m^2/g]
T	Tensile index [Nm/g]
w	Mass share (of a component/fraction) [%]
WI	Fibre width [µm]
ZI	Zero-span tensile index [Nm/g]

2 MFC trials at PTS

2.1 Materials

2.1.1 Fibrous raw materials

Pulp

The pulp used in the study was a mixture of 80 % ECF-bleached hardwood (*eucalyptus glob.*) and 20 % ECF-bleached softwood pulps. The pulp was refined using the pilot refiner at PTS under following conditions:

- SRE 65 kWh/t
- SEL 0,1 Ws/m

Fibre properties

For analyzing pulp fibres a FIBERLAB 3.0 device was used.

Tab. 1: Fibre properties of the used hardwood/softwood pulp mixture according to the FIBERLAB Protocol

Parameter	Unit	Value
Fines(numerically weighted)	%	12,58
Fines(length weighted)	%	2,17
Mean fibre length (numerically weighted)	mm	0,61
Mean fibre length (length weighted)	mm	0,86
Mean fibre length (length^2 weighted)	mm	1,27
Width	µm	16,30
Cell wall thickness	µm	3,54
Curl	%	17,30
Coarseness	mg/m	0,07

A special method was used to characterize the fibre fraction and dimensions of collapsed and dried fibres in the fibre network (see [5], [8])

Tab. 2: Properties of the fibre fraction and fibre dimensions after collapsing and drying

Parameter	Symbol	Unit	Value
Fibres (mass)		%	95,66
Fibre length	*FL*	mm	0,60
Fibre width	*WI*	µm	15,96
Cell wall thickness	*CWT*	µm	2,96
Fibre diameter (collapsed/dried)	*D*	µm	7,98
Fibre height (collapsed/dried)	*H*	µm	2,96

2.1.2 Additives

MFC

The Microfibrillated cellulose (MFC) used was delivered by STFI (code batch 004007/009). Properties and preparation procedure of MFC are summarised in the D2.24 Report on characterisation of Standard MFC. [2]

All MFC trials were carried out with 1%, 3%, and 5 % additions of MFC based on dry pulp.

Retention agent

The trials were carried out without retention agent and with the high-molecular cationic polymer Polymin SK (PEI). PEI was added at 0.25 % based on dry pulp. Also different trials were carried out with 0.25 % PEI based on dry MFC.

2.2 Methods

2.2.1 Technical methods

MFC preparation

The MFC used was stirred for 10 minutes at 2 g/l consistency and treated with an ultra-turrax blender for 2 minutes.

Sheet forming and addition of additives

Sheets were formed in a Rapid Köthen former according to ISO 5269-2. 2 g/l MFC were added to the stock container of the Rapid Köthen sheet per sheet, to a pulp consistency of 3 g/l. When PEI was used as retention agent, it was also added in the stock container after the MFC addition.

This procedure was close to the conditions prevailing in an approach flow system.

Testing methods for sheet properties

Tab. 3: Testing methods for sheet properties

Sheet properties	Standard/Method
Grammage	ISO 536
Thickness	ISO 534
Apparent density	ISO 534
Breaking length	ISO 1924-2
Tensile index	ISO 1924-2
Elongation	ISO 1924-2
Elastic modulus	ISO 1924-2
Tensile energy absorption index	ISO 1924-2
Tearing resistance (Brecht Imset)	DIN 53 115
Air permeability (Gurley)	ISO 5636-5
Internal bond (Scott Bond)	TAPPI T-833
Brightness	DIN 53145-T01-00
Spec. light scattering coefficient	DIN 54500-96
Spec. light absorption coefficient	DIN 54500-96

2.2.2 Mathematical methods

Correlation between SR value and specific surface area

The following formula was used to estimate the (hydrodynamic) specific surface area of a pulp from a given SR value

$$SSA = c_{SSA} \cdot \sqrt{\frac{SR - 4}{100 - SR}} \qquad (\ 2\text{-}1\ )$$

where

SSA: Specific surface area [m^2/g]
SR: SCHOPPER-RIEGLER value [°]
c_{SSA}: Factor depending on pulp viscosity, among other

The formula takes into account that

- SSA=0 for pure water (SR=4)
- SSA=∞ for a totally non-drainable pulp (SR=100)

The factor c_{SSA} is about 6,24 when applying known corresponding values of SR and SSA from HEINEMANN [3,4]. Formula (2-1) is only valid if no chemical additives are used which could influence the pulp viscosity.

The SSA value is additive. If SSA_{Pulp} / SSA_{MFC}, are the specific surface areas of the pulp / microfibrillated cellulose and w_{MFC} is the mass-weighted MFC share then the specific surface area SSA_{Total} of the pulp-MFC mix is

$$SSA_{Total} = (100\% - w_{MFC}) \cdot SSA_{Pulp} + w_{MFC} SSA_{MFC} \qquad (\ 2\text{-}2\ )$$

A similar equation (2-3) is valid if we use the specific surface areas SSA_{Total} of the pulp before sheet forming, SSA_{Ret} of the retained pulp, which is obtained by disintegrating the formed fibre mat before drying and pressing, and SSA_{Unret} of the non-retained pulp.

$$SSA_{Total} = w_{\mathrm{Re}t} SSA_{\mathrm{Re}t} + (100\% - w_{\mathrm{Re}t}) \cdot SSA_{Unret} \qquad (\ 2\text{-}3\ )$$

Here w_{Ret} is the mass weighted share of the retained pulp.

Simplified fibre network as reference

To estimate the relative bonded area RBA (a critical value for applying the PAGE equation) in a given sheet, one can use a regular fibre network (*Fig. 1*) reference which is made up of the same fibres and which has the same apparent density like the original fibre network.

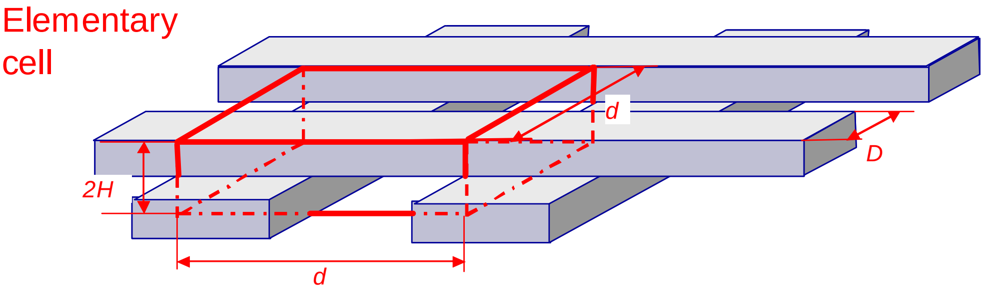


Fig. 1: Regular fibre network with elementary cell

After calculating the values *D* (diameter) and *H* (height) of the collapsed and dried fibres in the network from the fibre width *WI* and cell wall thickness *CWT* of fibres in the suspension (for more details see [5]), we have yet to calculate the distance *d* (distance of neighbouring fibres in a layer, which equals the length and width of the elementary cell) according to (2-4). Equation (2-4) ensures that the apparent density of the elementary cell equals the apparent density ρ of the sheet.

$$d = \frac{D \cdot \rho_W}{AD} \qquad (2\text{-}4)$$

The density ρ_W of the fibre wall material is about 1,5 g/cm^3 [6].

RBA

Calculating the relative bonded area (RBA) is now trivial. Using the total fibre surface A_T area per elementary cell

$$A_T = 4d \cdot D + 4d \cdot H \qquad (2\text{-}5)$$

and the bonded fibre surface A_B area per elementary cell

$$A_B = 4D^2 \qquad (2\text{-}6)$$

yields

$$RBA = \frac{A_B}{A_T} \qquad (2\text{-}7)$$

Bonding strength

Bonding strength *b* can now be calculated via the Page equation (2-8) [6] for given values of mean fibre length *FL*, tensile index *T* and zero-span tensile index *ZI*. The cross sectional fibre area A_{CSA} equals $D \cdot H$ and the fibre perimeter *P* equals 2(*D*+*H*).

$$\frac{1}{T} = \frac{9}{8ZI} + \frac{12 \cdot A_{CSA} \cdot \rho_W}{b \cdot P \cdot FL \cdot RBA} \qquad (2\text{-}8)$$

2.3 Results

2.3.1 Physical paper properties (Overview)

Tab. 4: Physical paper properties of the reference pulp and pulp with MFC-2

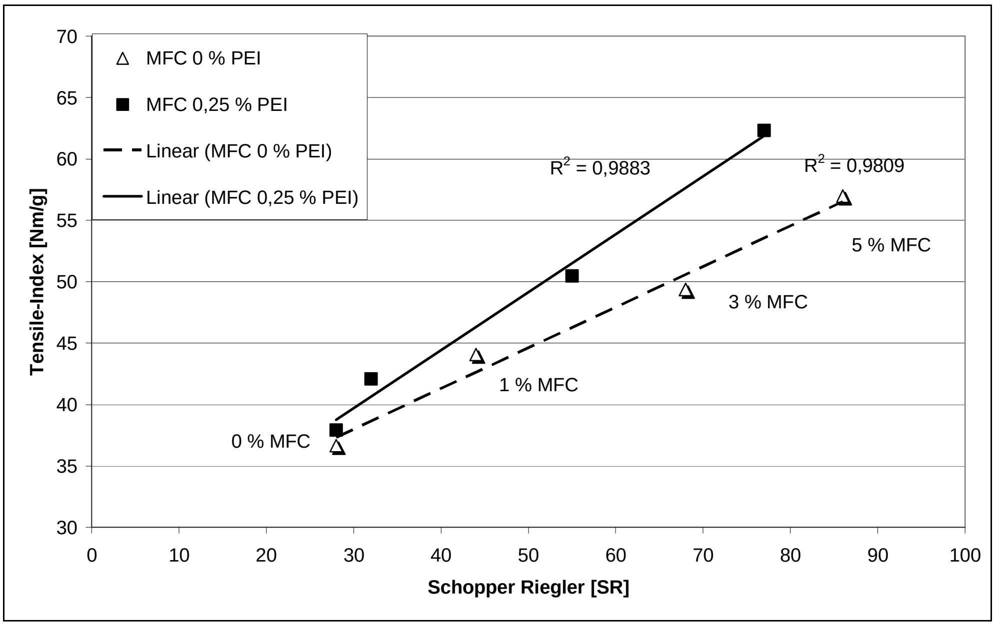
MFC	%	0,00%	1,00%	3,00%	5,00%	0,00%	1,00%	3,00%	5,00%
PEI on dry pulp	%	0,00%	0,00%	0,00%	0,00%	0,25%	0,25%	0,25%	0,25%
SR	°	28	44	68	81	28	32	55	77
Grammage	g/m^2	79,74	79,98	78,94	82,31	82,46	80,00	79,77	84,22
Apparent Density	g/cm^3	0,61	0,60	0,62	0,66	0,59	0,62	0,63	0,66
Air permeability	ml/min	1873	603	185	25	1924	1203	214	19
Tensile Index	Nm/g	36,66	44,08	49,37	56,97	37,91	42,09	50,46	62,33
TEA Index	J/g	0,74	1,04	1,18	1,46	0,78	1,06	1,35	1,69
E-Modulus	Mpa	3430	3656	4096	4520	3353	3547	4074	4863
Tensile Stiffness I.	kNm/g	5,58	6,07	6,63	6,84	5,69	5,74	6,51	7,37
Scott Bond	J/m^2	229	345	421	453	305	223	463	551
Elongation	%	2,65	3,12	3,17	3,41	2,69	3,33	3,53	3,63
Tearing resistance	mNm/m	1275	1447	1533	1724	1349	1422	1576	1833
Brightness	%	88,92	88,87	88,38	87,23	85,96	84,15	85,50	83,89
Opacity	%	81,28	80,95	80,06	79,31	83,33	84,71		81,51
Light absorption	m^2/kg	0,11	0,11	0,12	0,13	0,23	0,32	0,22	0,27
Light scattering	m^2/kg	40,60	39,82	37,12	34,30	39,14	40,34	36,83	33,63

Tensile index and SR

After adding MFC-2 the tensile index was increased. A clear linear correlation could be observed between tensile index and SR value. With 5 % MFC-2 the tensile index had been increased from 36,6 to 62,3 Nm/g. As you can see in *Fig. 2*, adding a small amount of PEI as retention agent has improved the impact of MFC-2 on tensile-index.

Influence of MFC on tensile index

Fig. 2: Influence of MFC-2 on the tensile index



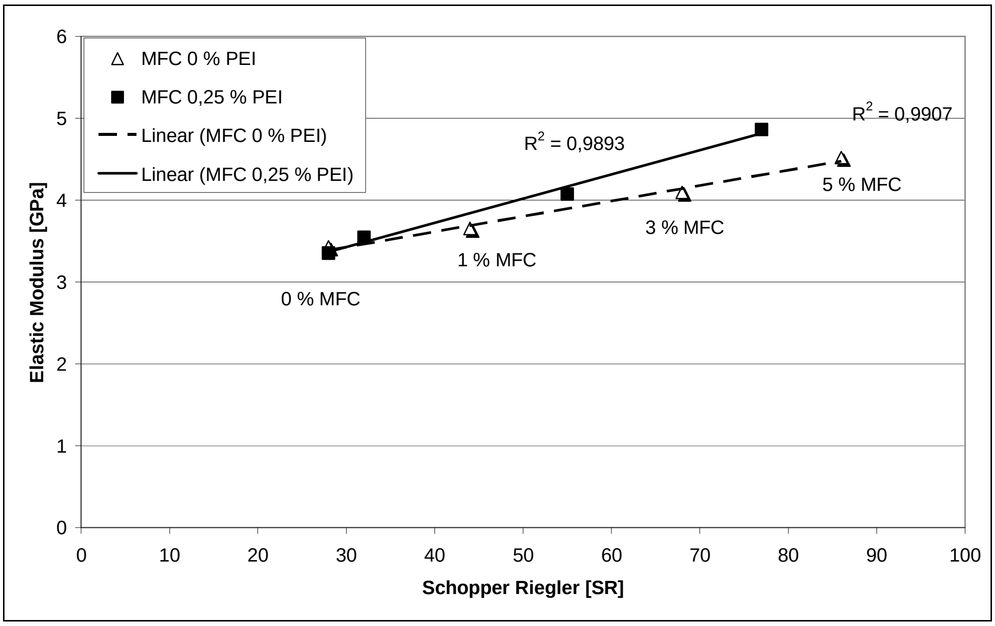
E-modulus

The E-modulus is one of the most crucial factors for the top layer of 3-layer packaging board. *Fig. 3* shows the development of E-modulus with the additions of MFC-2.

The same tendency of E-modulus versus tensile index is evident. With 5 % MFC-2, the E-modulus of the pulp was about 42 % higher than that of the pulp without MFC. The best results were achieved when using a low amount of PEI.

Influence of MFC on E-Modulus

Fig. 3: Influence of MFC-2 on E-modulus

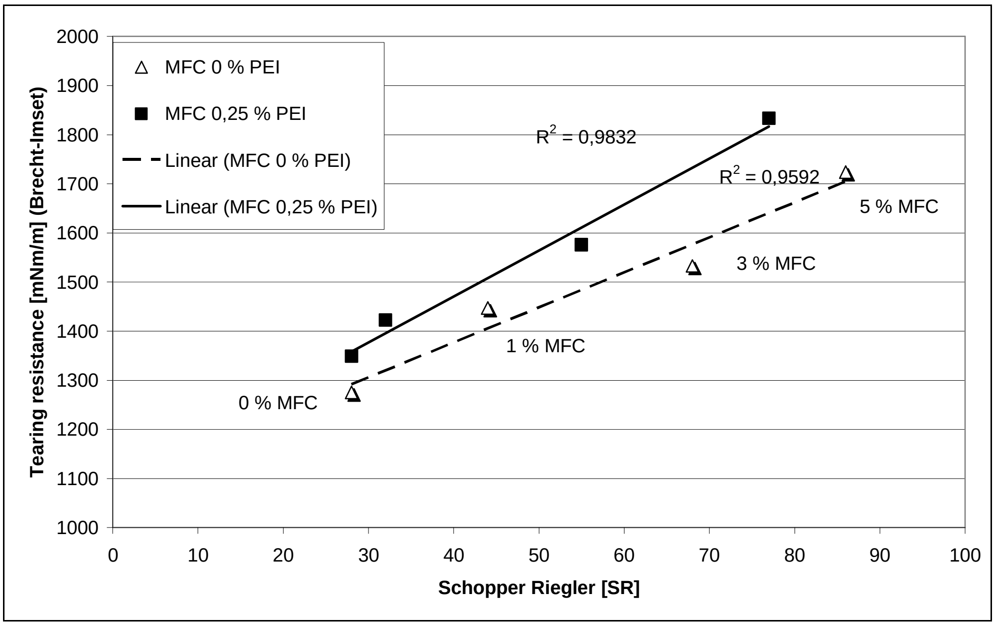


Tearing resistance

The tensile index reflects the degree of fibre bonding due to the relative bonding area. Tearing resistance depends mostly on fibre length and on the bonding strength between fibres. *Fig. 4* shows the SR value plotted against the tearing resistance. It can be seen that the tearing resistance is enhanced by MFC as well. The tearing resistance was increased to about 44 %, and an efficient application of MFC-2 is evidently supported by PEI because the tearing resistance was higher with PEI and MFC-2 than with MFC-2 and no PEI addition.

Influence of MFC-2 on tearing resistance (Brecht-Imset)

Fig. 4: Influence of MFC-2 on tearing resistance (Brecht-Imset)

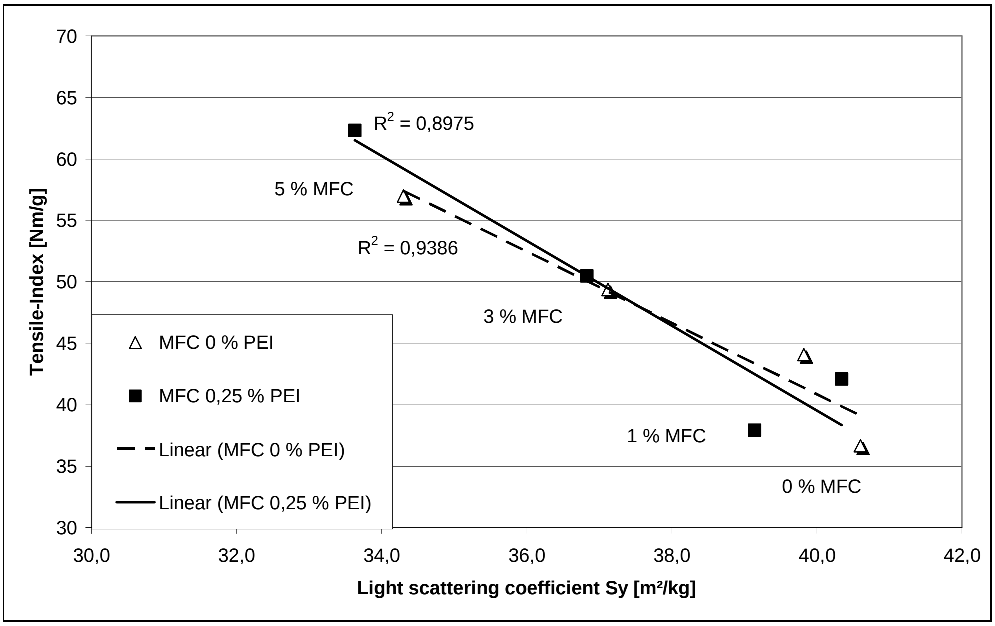


Light scattering coefficient

The light scattering coefficient depends on the apparent density of a paper sheet and reflects the relative bonding area of fibres. At higher light scattering coefficients, the light is scattered more due to higher amounts of unbonded areas in the sheet. *Fig. 5* shows that the S value (Y-spectral range) increases and the tensile index decreases. This indicates a higher relative bonding area due to the application of MFC-2. This higher relative bonding area leads to a higher tensile index.

Influence of MFC-2 on light scattering coefficient and tensile index

Fig. 5: Influence of MFC-2 on light scattering coefficient and tensile index



2.3.2 Properties and retention of MFC-2

Specific surface area of MFC-2

Tab. 5 lists the SR values measured before sheet forming (SR_{Total}) and after disintegration (SR_{Ret}) for different MFC-2 dosages and PEI additions. The corresponding specific surface areas SSA_{Total} and SSA_{Ret} , calculated according to (2-1), have been included in the table as well, but only for those samples were no retention aid was used. SSA_{MFC} were calculated via (2-2). The specific surface area of the MFC-2 used here is about 180 m^2/g.

SCHOPPER-RIEGLER values and specific surface areas for different additions of MFC-2 and PEI

Tab. 5: SCHOPPER-RIEGLER values and specific surface areas for different additions of MFC-2 and PEI

w_{MFC}	PEI (to MFC)	PEI (to Pulp)	SR_{Total}	SR_{Ret}	SSA_{Total}	SSA_{Ret}	SSA_{MFC}
%	%	%	°	°	m^2/g	m^2/g	m^2/g
0,00%	0,00%	0,00%	28	26	3,60	3,40	-
1,00%	0,00%	0,00%	44	33	5,27	4,11	170,71
3,00%	0,00%	0,00%	68	55	8,82	6,64	177,67
5,00%	0,00%	0,00%	81	n.a.	12,56	-	182,79
0,00%	0,00%	0,25%	28	n.a.	3,60	-	-
1,00%	25,00%	0,25%	32	27	4,00	3,50	-
3,00%	8,30%	0,25%	55	n.a.	6,64	-	-
5,00%	5,00%	0,25%	77	72	11,12	9,72	-
3,00%	25,00%	0,75%	64	51	8,06	6,11	-
5,00%	25,00%	1,25%	48	37	5,74	4,52	-

MFC-1

Application of formula (2-2) on the *SR* values of the first trials reported in [1] yields a specific surface area of about 30 m^2/g for MFC-1, which is significantly lower than the average value for MFC-2

Tab. 6: SCHOPPER-RIEGLER values and specific surface areas for different pulp grades after addition of 5% MFC-1

Pulp grade	*SRE*	*SR* (without MFC)	*SR* (with 5 % MFC-1)	SSA_{MFC}
	kWh/t	°	°	m^2/g
Birch	50	22	32	23,1
Birch	100	37	48	29,0
Softwood	50	23	35	27,3
Softwood	100	32	38	38,7

MFC retention

In *Fig. 6* corresponding values of SSA_{Total} and SSA_{Ret} are plotted in one diagram. The points can be perfectly connected by a straight line. The slope of the line is 0,6353 - which means that for all 3 samples at most 63,5% of MFC-2 is retained in the sheet. The dotted line represents identical values of SSA_{Total} and SSA_{Ret} or in other words the fully retention of MFC.

In the following we will see that due to the addition of MFC also more fines seem to be retained.

***SSA_{Total}* vs. *SSA_{Ret}*.**

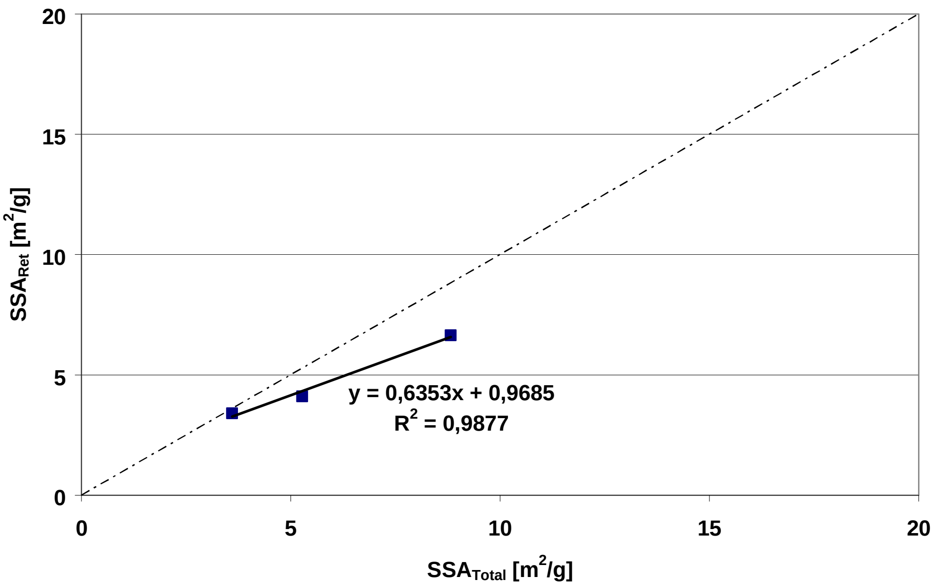


Fig. 6: Specific surface areas of Pulp-MFC-2 blends without PEI

2.3.3 Apparent density

According to *Fig. 7* the apparent density increases by 0,012 g/cm^3 or 2% per addition of another 1% MFC-2. Compared to the MFC-1 results in [1] with growth rates of 0,5% (hardwood) and 0,1% (softwood), the increase in apparent density is significantly higher for MFC-2 than for MFC-1. Because the ratio of the rates is nearly the same as the ratio of the MFC specific surface areas, the following relation will be used for modelling to predict the apparent density after MFC addition:

$$AD = AD_0 + \frac{SSA_{MFC}}{142} w_{MFC} \qquad (2\text{-}9)$$

where

AD_0: Apparent density before MFC addition [g/cm^3]
AD: Apparent density after MFC addition [g/cm^3]
SSA_{MFC}: Specific surface area of the MFC used [g/m^2]
w_{MFC}: MFC share [%]

It is almost certain that the increase in apparent density is solely due to the incorporation of more MFC and fines particles into the voids of the fibrous backbone. If we assume that the retention rate of MFC is about 50% (see *Fig. 6*), then only 0,5% of the 2% density increase (per 1% MFC-2 addition) are due to MFC whilst the remaining 1,5% are likely to be due to improved fines retention.

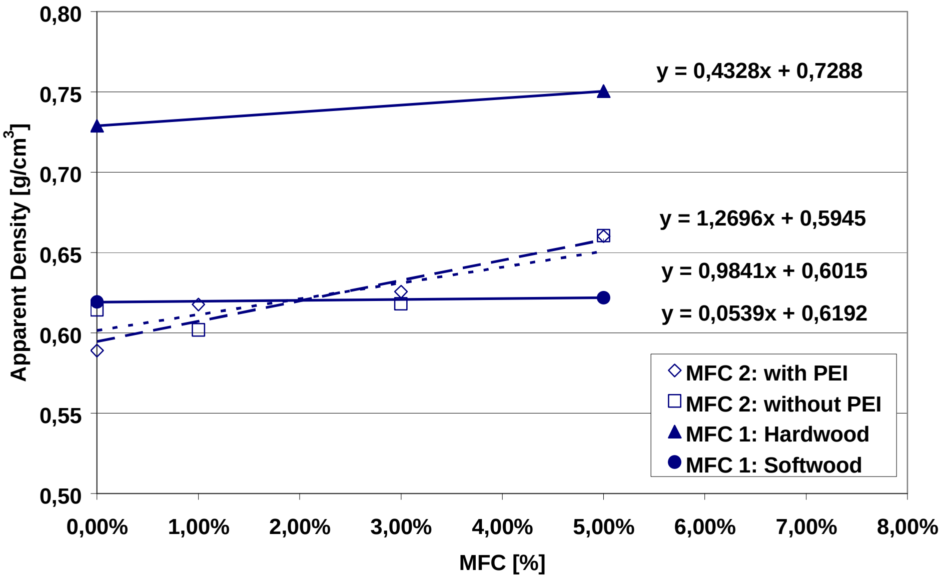


Fig. 7: Increase in apparent density by MFC addition

2.3.4 Bonding strength

Simplified reference fibre network data

Tab. 7 contains the basic data of the simplified reference fibre networks after applying the formulas (2-4)to (2-8) on the fibre characteristics (*Tab. 2*) and the tensile indices and apparent densities measured in lab sheets.

Basic data of the simplified reference fibre network

Tab. 7: Basic data of the simplified reference fibre network.

w_{MFC}	PEI (MFC)	PEI (Pulp)	A_T	A_B	d	RBA	$b^{1)}$
%	%	%	μm^2	μm^2	µm		MPa
0,00%	0,00%	0,00%	871,41	254,67	19,91	0,29	4,76
1,00%	0,00%	0,00%	889,54	254,67	20,33	0,29	6,43
3,00%	0,00%	0,00%	866,13	254,67	19,79	0,29	7,52
5,00%	0,00%	0,00%	810,62	254,67	18,53	0,31	9,00
0,00%	0,00%	0,25%	908,99	254,67	20,77	0,28	5,22
1,00%	25,00%	0,25%	866,65	254,67	19,81	0,29	5,83
3,00%	8,30%	0,25%	855,65	254,67	19,55	0,30	7,70
5,00%	5,00%	0,25%	811,00	254,67	18,53	0,31	10,62
3,00%	25,00%	0,75%	857,42	254,67	19,59	0,30	7,92
5,00%	25,00%	1,25%	856,56	254,67	19,57	0,30	6,35

1) A zero-span tensile index of 150Nm/g was assumed according to [7] for calculating b with (2-8)

Improvement of bonding strength by MFC

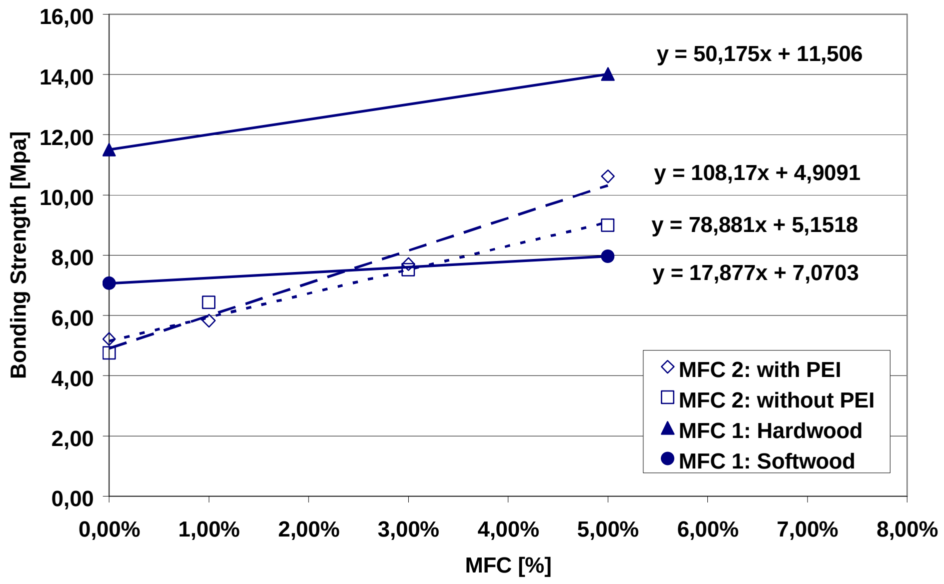


Fig. 8: Improvement of bonding strength by MFC

Dependence between MFC grade and bonding strength growth rate

The ratio of bonding strength growth rates between MFC-1 and MFC-2 per 1 % addition of MFC is nearly the same as the ratio of MFC-induced specific surface areas between the two MFC grades. This leads to the following approximation of the dependency between bonding strength levels before and after MFC addition

$$b = b_0 + \frac{SSA_{MFC}}{1{,}76} w_{MFC} \qquad (2\text{-}10)$$

where

b_0: Bonding strength before MFC addition [MPa]
b: Bonding strength after MFC addition [MPa]

2.3.5 Elastic modulus and Scott Bond

Basic properties for WP 2.2

In respect of the paper properties which are important for WP 2.2 it is interesting to visualize the dependencies of elastic modules and Scott Bond values on the bonding strength values of fibres (*Fig. 9* and *Fig. 10*).

Obviously both parameters seem to be nearly independent of pulp, MFC and additive use. Furthermore the relations are of a clearly linear type.

Bonding strength vs. E- modulus

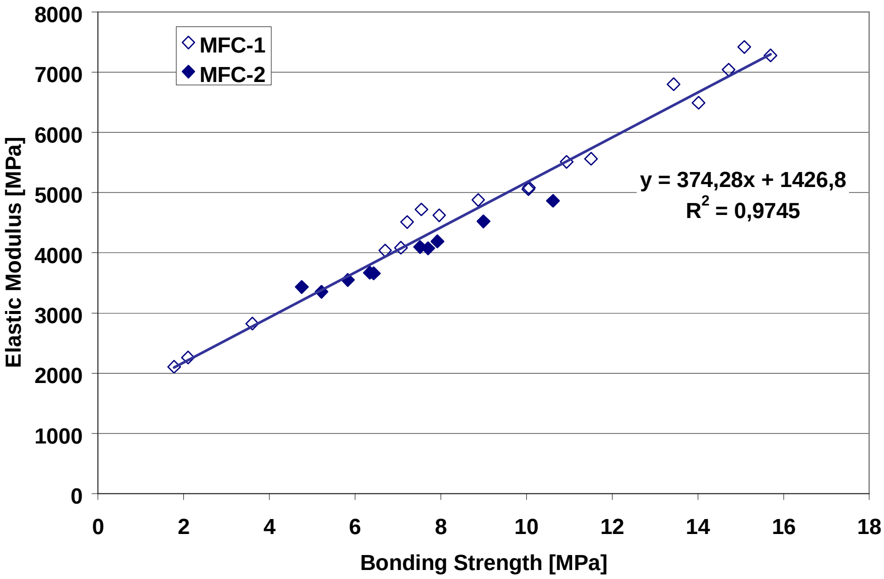


Fig. 9: Bonding strength vs. Elastic modulus and Scott Bond for various additions of MFC

Bonding strength vs. Scott Bond

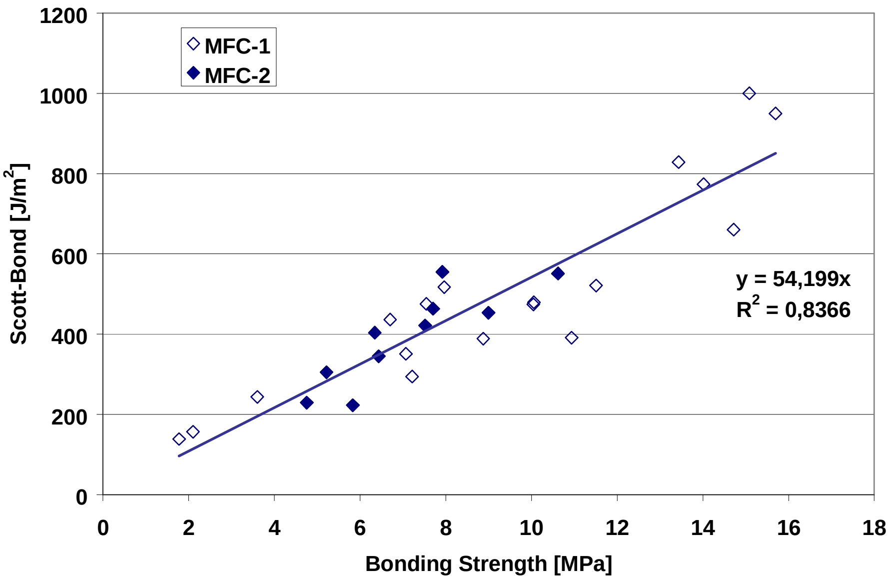


Fig. 10: Bonding strength vs. elastic modulus and Scott Bond for various additions of MFC

Elastic modulus

The intersection of the regression line (*Fig. 9*) with the ordinate yields the value of the elastic modulus for the "unbonded" fibre network or, in other words, the elastic modulus of single fibres is about 1427 MPa.

The slope of the regression line in *Fig. 9* is 374 (MPa/MPa). Thus, the following relation can be used to predict the elastic modulus after MFC addition:

$$EM = EM_0 + 374 \cdot b(w_{MFC}) \qquad (2\text{-}11)$$

where

EM_0: Elastic modulus before MFC addition [MPa]
EM: Elastic modulus after MFC addition [MPa]
$b(w_{MFC})$: Increase in bonding strength due to the addition of MFC

Scott Bond

Because a network containing no bonded fibres implicates no strength in z-direction, the regression line and their slope (54 Jm^{-2}/MPa) was calculated under the constraint that the additive constant is zero or, in other words, the regression line intersects the point of origin. Consequently the following equation will be used for the prediction of Scott-Bond. The related formula for Scott Bond prediction is

$$SB = SB_0 + 54 \cdot b(w_{MFC}) \qquad (2\text{-}12)$$

where

SB_0: Scott Bond before MFC addition [J/m^2]
SB: Scott Bond after MFC addition [J/m^2]

3 Numerical simulations for a 3-layered board

Final equations

Using

$$b(w_{MFC}) = b(w_{MFC}) - b_0 \qquad (3\text{-}1)$$

from (2-10),(2-11) and (2-12) the following final equations can be derived

$$EM = EM_0 + 212{,}5 \cdot SSA_{MFC} \cdot w_{MFC} \qquad (3\text{-}2)$$

$$SB = SB_0 + 30{,}7 \cdot SSA_{MFC} \cdot w_{MFC} \qquad (3\text{-}3)$$

which directly relate the increase in elastic modulus and Scott Bond to the amount and the quality of MFC used.

Model structure

A general model structure was presented in [8]. In order to include the addition of MFC the following modification was made:

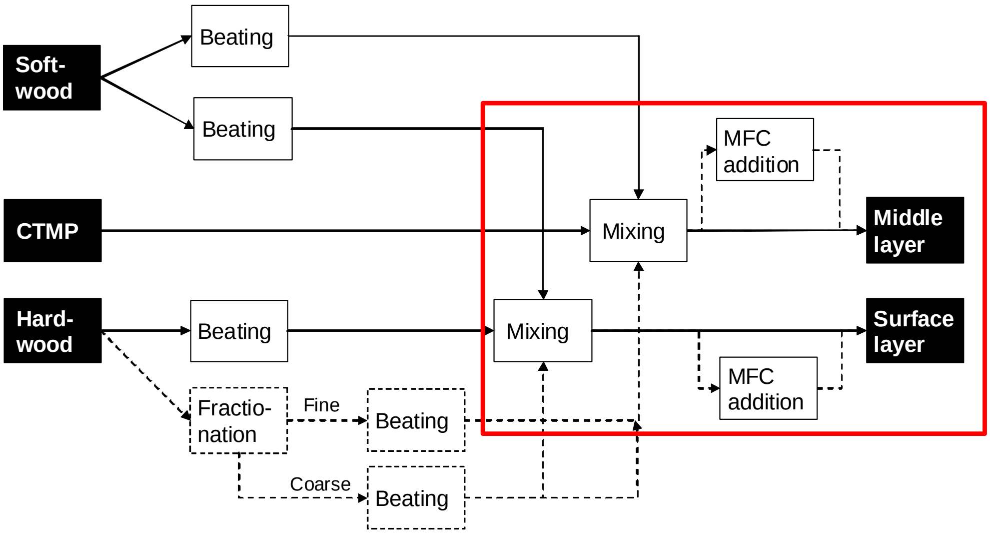


Fig. 11: Basic model structure. The frame delimits the process section which is the focus of this report

Focus of simulation

Because all the other processes have already been simulated in various combinations the focus of the recent simulation was on applying the process steps (MFC addition in the layers) within the frame visualized in *Fig. 11*. The simulation starts with the values after mixing.

Reference board

In [8] the following data were used as reference for top/back layers and the middle layer.

Tab. 8: Reference values for a symmetrical 3-layered board

Top/back layers	Basis weight	g/m^2	100,00
	SR	°	26,17
	AD	g/cm^3	0,78
	EM	MPa	6123,47
	SB	J/m^2	419,81
Middle layer	Basis weight	g/m^2	150,00
	SR	°	27,63
	AD	g/cm^3	0,48
	EM	MPa	2477,03
	SB	J/m^2	51,01
Critical paper properties of the board	Basis weight	g/m^2	250,00
	BS	mNm	34,36
	SB	J/m^2	51,01

Expansion of the simulation model

As in [8] the critical paper properties of a multilayered board can be calculated as follows:

- *Bending stiffness:* Calculated according to the laminate theory [9]
- *z-strength [J/m^2]:* The value of z-strength equals the minimum of the individual values in each layer[1]

For calculating the effects of MFC addition the formulas (2-1),(2-2),(2-9), (3-2) and (3-3) can be used.

Constraints for the EXCEL-solver

The numerical model was implemented into an EXCEL sheet. For calculation and optimisation the EXCEL solver was used with the following 4 different sets of constraints (#1, #2, #3, #4) for a 3 layered board:

- Bending Stiffness ≥ 34,36 mNm (#1, #2, #3, #4)
- z-strength ≥ 51,01 J/m^2 (#1, #2, #3, #4)
- SR values in the layers ≤ 50°(#1, #4), 65°(#2), 80°(#3)
- Addition of MFC was limited to 5% (#1, #2, #3, #4)
- Specific surface area of MFC ≤ 180 m^2/g (#1, #2, #3), 30m^2/g (#4)

The optimization results are summarized in *Tab. 9*.

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[1] The real value is more likely to be somewhere between the values of the surface layer and middle layer.

Simulation results

Tab. 9: Results of the optimised simulation model

	Trial	Ref	#1	#2	#3	#4
Total						
Basis weight	g/m^2	250,00	244,50	241,66	237,26	245,97
BS	mNm	34,36	34,36	34,36	34,36	34,36
SB	J/m^2	51,01	51,01	51,01	51,01	51,01
Middle layer						
Basis weight	g/m^2	150,00	171,40	167,04	161,18	173,89
SR	°	26,17	26,17	26,17	26,17	26,17
AD	g/cm^3	0,48	0,48	0,48	0,48	0,48
EM	MPa	2477,03	2477,03	2477,03	2477,03	2477,03
SB	J/m^2	51,01	51,01	51,01	51,01	51,01
w_{MFC}	%	0,00	0,00	0,00	0,00	0,00
SSA_{MFC}	m^2/g	0,00	0,00	0,00	0,00	0,00
Top/back layer						
Basis weight	g/m^2	100,00	71,42	71,49	70,49	71,12
SR	°	27,63	50,00	65,00	80,00	40,50
AD	g/cm^3	0,78	0,80	0,82	0,84	0,79
EM	MPa	6123,47	6698,95	7197,92	8067,55	6455,72
TSI	kNm/g	7,84	8,38	8,83	9,57	8,16
SB	J/m^2	419,81	499,57	568,73	689,26	465,86
w_{MFC}	%	0,00	5,00	5,00	5,00	5,00
SSA_{MFC}	m^2/g	0,00	51,96	97,02	175,54	30,00

Discussion of the simulation results

Obviously some trends are clearly visible:

- MFC should primarily be used in the top and back layers
- The basis weights of top and back layers can be decreased symmetrically whereas the middle layer basis weight should be increased

Some extra simulations show that in order to prevent an “overflow” of SR values some alternative strategies can be adopted. The same result as in #2 can be achieved, for example, by using a “better” MFC quality (SSA_{MFC}=180 m^2/g) but at lower amount (w_{MFC} =2,65%)

SR values

The most limiting factor for the use of MFC in top and back layers is the increase in SR value as a result of MFC addition. The SR values listed above are calculated without consideration of a retention aid which is likely to reduce the dewatering resistance. Depending on which SR value is acceptable for top/back layers the total weight of the 3-ply board can be decreased by adding 2-6 % MFC whilst maintaining given levels of z-strength and bending stiffness.

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