

Supplementary Materials

Fast and efficient method to evaluate the potential of eutectic solvents to dissolve lignocellulosic components

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S1 – THERMO ANALISYS

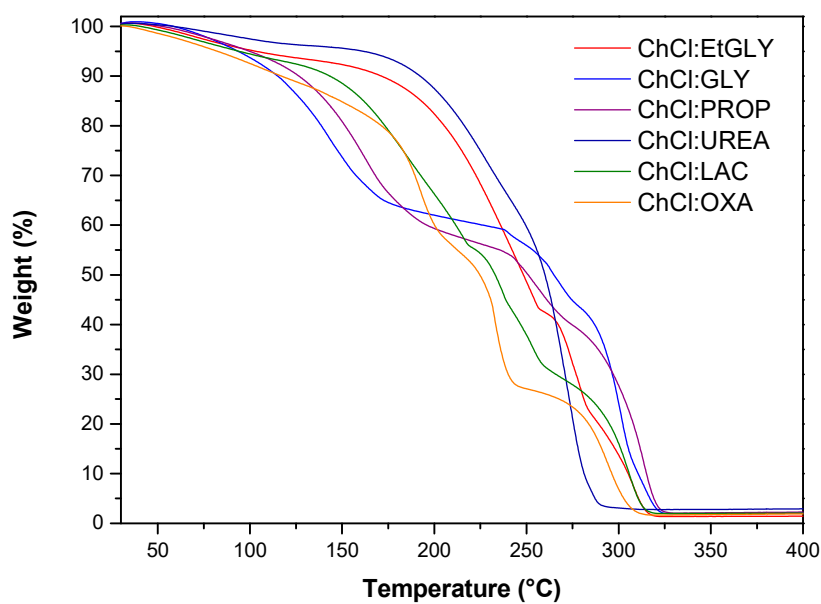


Figure S1. TGA thermograms of studied ES.

S2 – WATER CONTENT

Table S1. ES water content determined by Metrohm 831 Karl Fischer coulometer. Experiments were performed in triplicate. Viscosity and density values are given from literature reports.

ES	Water Content (wt%)	Viscosity η_a /mPa·s	Density g.cm ⁻¹
ChCl:EtGLY	3.22 ± 0.08	30.90 ¹	1.1146 ²
ChCl:GLY	2.55 ± 0.01	246.80 ³	1.1895 ²
ChCl:PROP	2.62 ± 0.05	39.20 ⁴	1.0300 ⁴
ChCl:UREA	2.56 ± 0.07	527.28 ⁵	1.1945 ⁵
ChCl:LAC	4.98 ± 0.10	215.70 ⁶	1.1726 ⁶
ChCl:OXA	2.54 ± 0.02	585.28 ⁷	1.7181 ⁷

S3- OPTICAL MICROSCOPY IMAGES

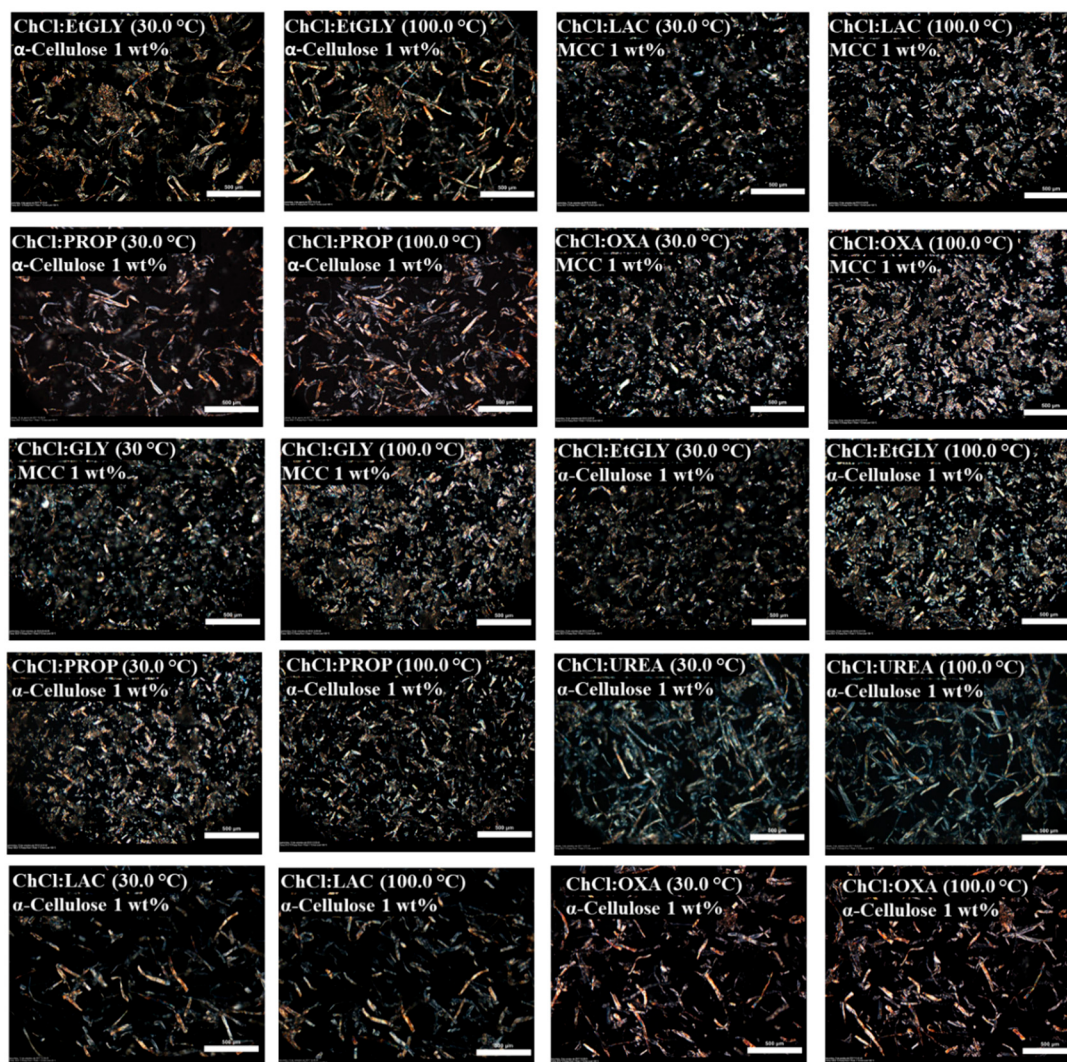


Figure S2. Images obtained by polarized optical microscopy of 1 wt% cellulose in ES at heating rate of 1 °C.min⁻¹ (magnification of 50x)

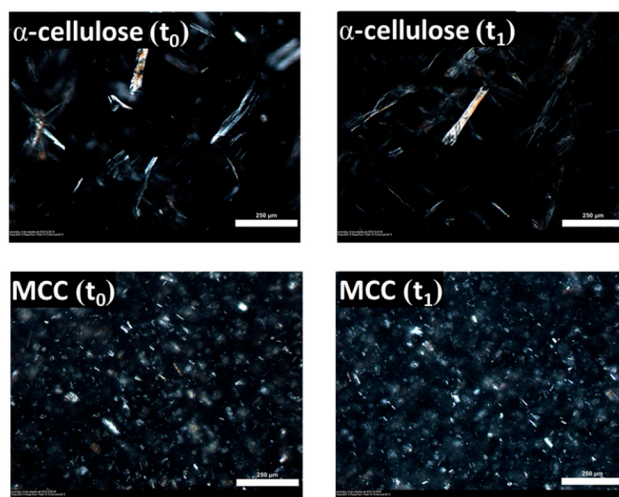


Figure S3. Polarized optical microscope images of 0.25 wt% MCC and α -cellulose suspension in ChCl:GLY at 60 °C after 48 hours of shaking (magnification of 50x).

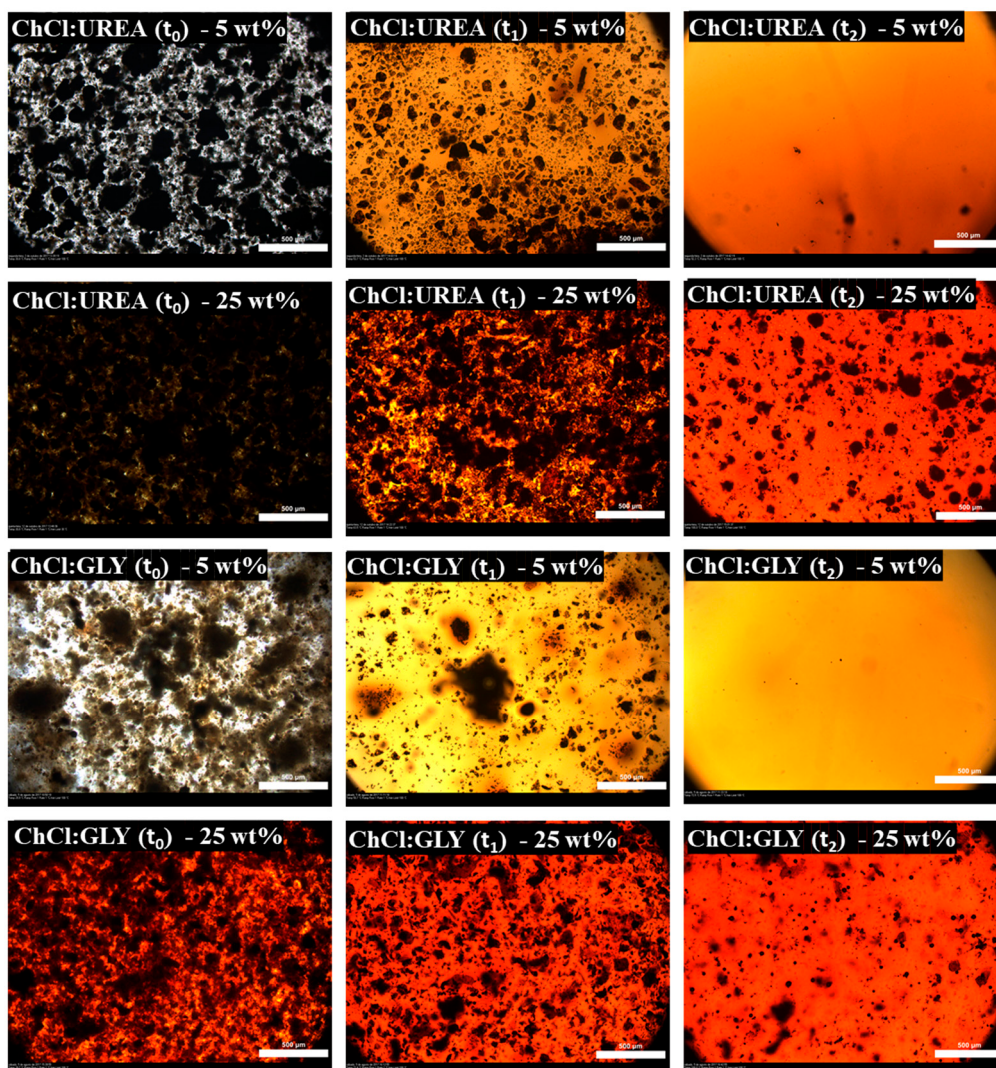


Figure S4. Images obtained by optical microscopy of 5 and 25 wt% lignin mass fractions in ES at heating rate of 1 °C.min⁻¹ (magnification of 50x).

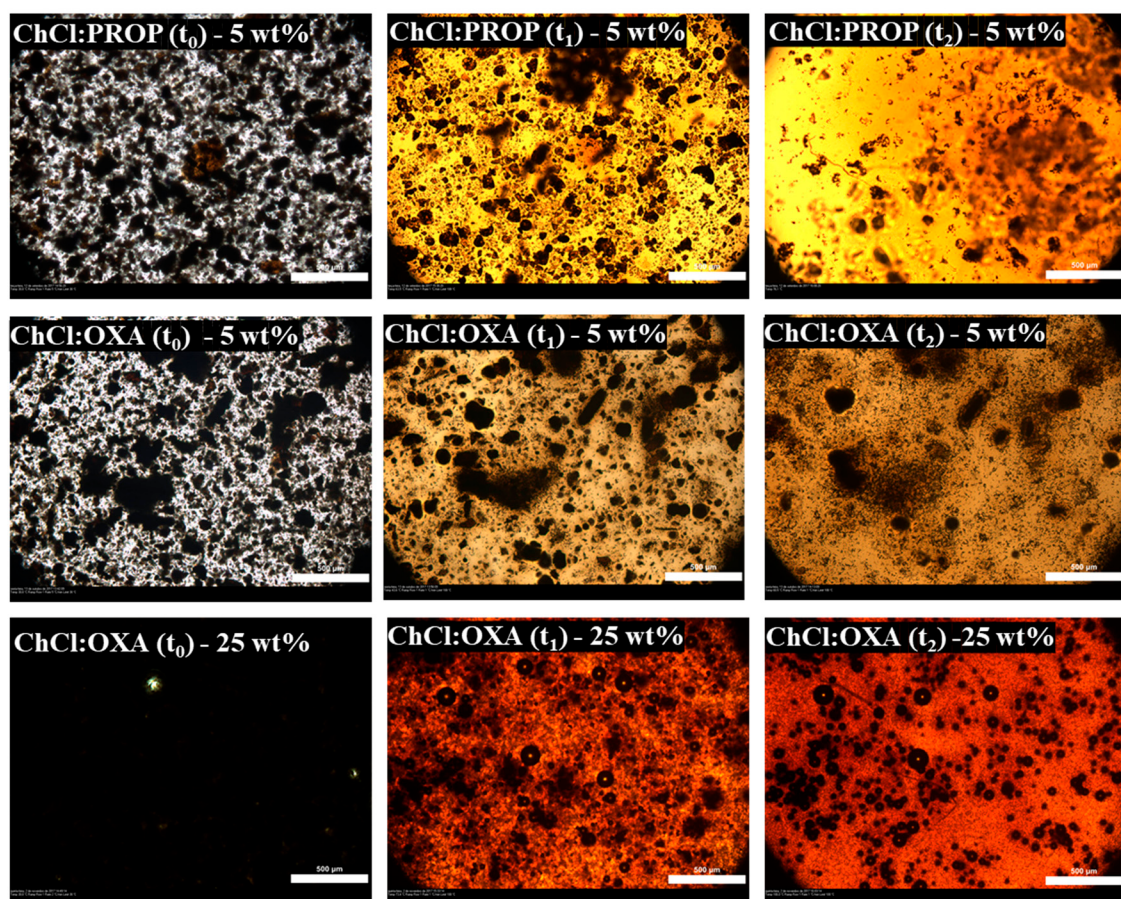


Figure S5. Images obtained by optical microscopy of 5 and 25 wt% lignin mass fractions in ES at heating rate of $1\text{ }^{\circ}\text{C}.\text{min}^{-1}$ (magnification of 50x).

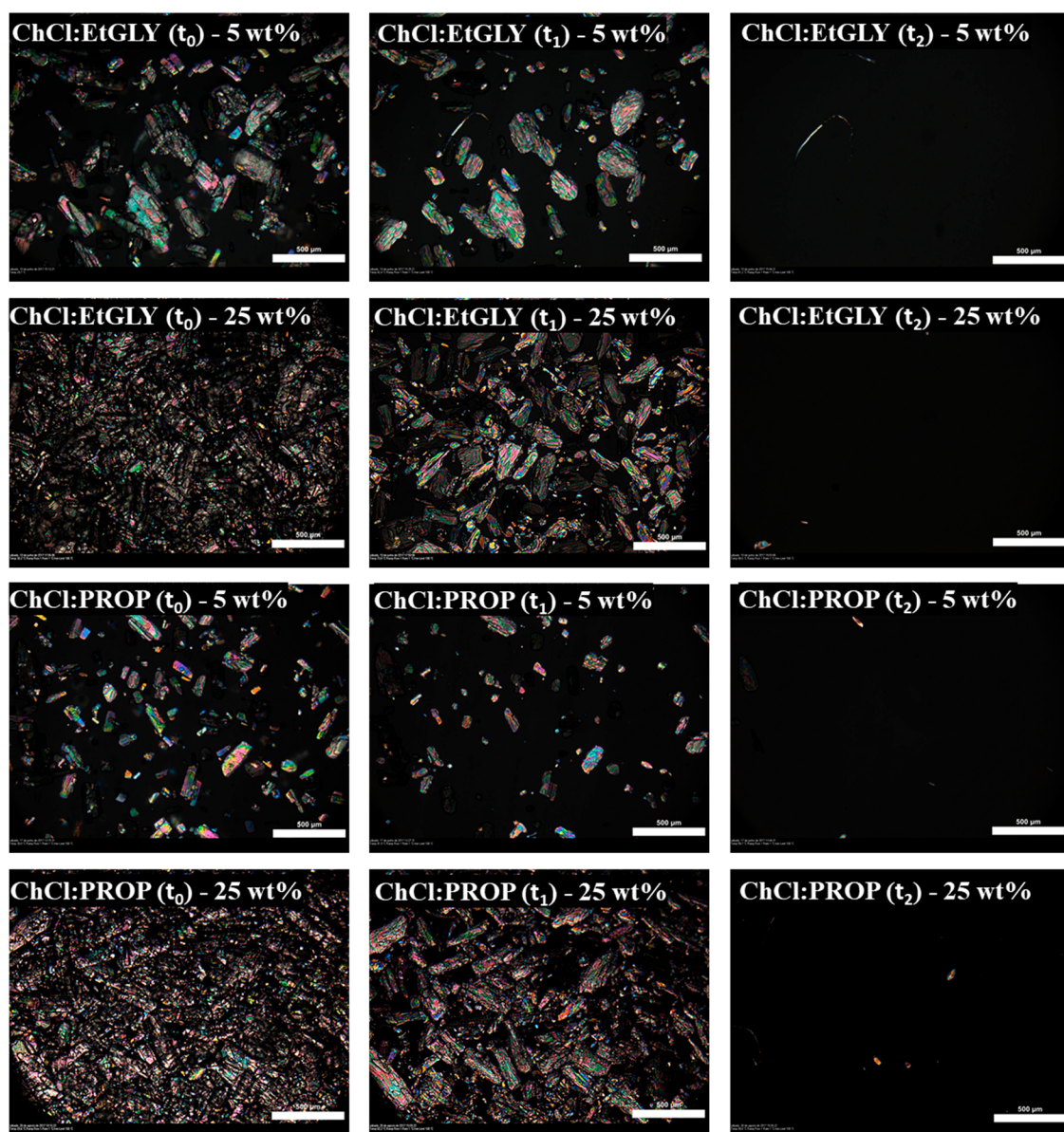


Figure S6. Images obtained by optical microscopy of 5 and 25 wt% xylose mass fractions in ChCl:EtGLY and ChCl:PROP at heating rate of $1\text{ }^{\circ}\text{C}.\text{min}^{-1}$ (magnification of 50x).

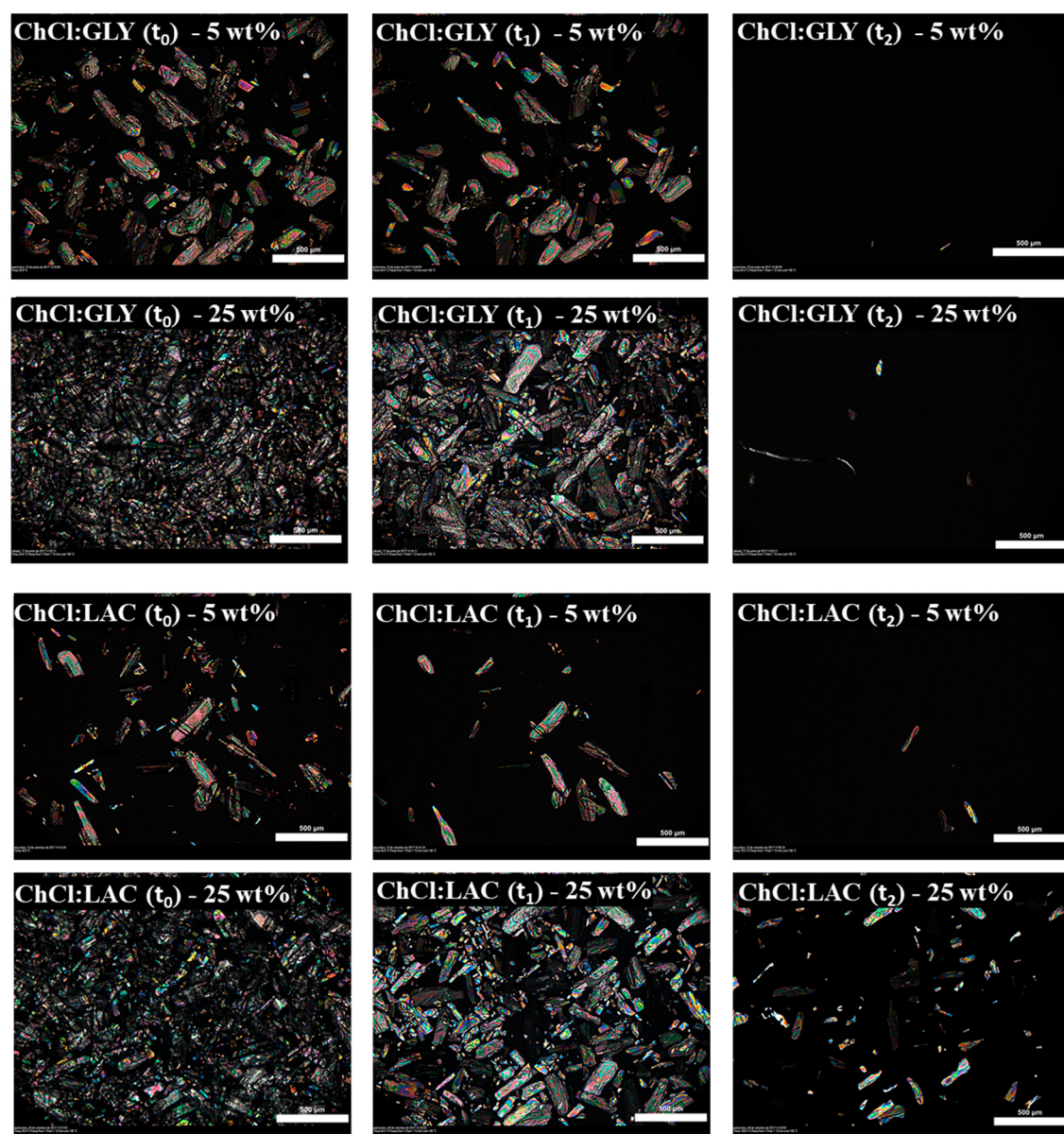


Figure S7. Images obtained by polarized optical microscopy of 5 and 25 wt% xylose mass fractions in ChCl:GLY and ChCl:LAC at heating rate of $1\text{ }^{\circ}\text{C}\cdot\text{min}^{-1}$ (magnification of 50x).

S4 – DISSOLUTION RESULTS

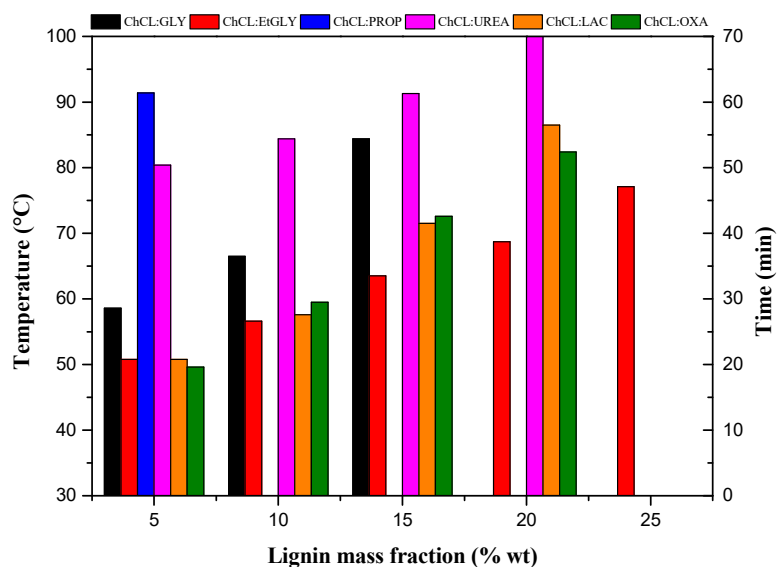


Figure S8. Time and temperature observed for complete dissolution of lignin in ES at heating rate of $1^{\circ}\text{C}.\text{min}^{-1}$.

Table S2. Temperature (and time) required for full dissolution of xylose in ES at different concentration. In each experiment the sample was heated from 30 to 100 $^{\circ}\text{C}$ at heating rate of $1^{\circ}\text{C}.\text{min}^{-1}$.

DES	5 wt% xylose		25 wt% xylose	
	Temperature	Time	Temperature	Time
ChCL:GLY	59.2 $^{\circ}\text{C}$	29.2 min	98.6 $^{\circ}\text{C}$	68.6 min
ChCL:EtGLY	46.9 $^{\circ}\text{C}$	26.9 min	98.3 $^{\circ}\text{C}$	68.3 min
ChCL:PROP	57.7 $^{\circ}\text{C}$	27.7 min	98.2 $^{\circ}\text{C}$	68.2 min
ChCL:UREA	59.6 $^{\circ}\text{C}$	29.6 min	83.3 $^{\circ}\text{C}$	53.3 min
ChCL:LAC	80.3 $^{\circ}\text{C}$	30.3 min	*	*
ChCL:OXA	61.5 $^{\circ}\text{C}$	31.5 min	96.6 $^{\circ}\text{C}$	66.6 min

* Did not occur the total dissolution until reaching the temperature of 100 $^{\circ}\text{C}$.

S5 – ESTIMATION OF MASS TRANSFER COEFFICIENT

The equation that describes the xylose mass decrease as a function of time can be represented as follows:

$$\frac{dm}{dt} = -|k_c|.s(m) \quad (1)$$

where $s(m)$ is the surface area of the xylose crystal for a given mass m and k_c is the mass transfer coefficient which is assumed to be constant.

In other words, the variation of the xylose mass in time is proportional to the surface area of xylose crystals. The surface area of xylose crystals was expressed as a function of a given mass (time dependent), which can be done due to the assumption of constant density. Considering the xylose crystals as a flat ellipsoid we can consider the following equations:

$$v(m) = \frac{4}{3} \cdot \pi \cdot a \cdot b \cdot c \quad (2)$$

$$s(m) \cong 2 \cdot \pi \cdot a \cdot b \quad (3)$$

$$\rho = \frac{m}{v} \quad (4)$$

considering that $a = x$; $b = 2x$; $c = 0.01x$

$$s(m) = 4 \cdot \pi \cdot \left(\frac{3m}{0.08\pi\rho} \right)^{2/3} \quad (5)$$

Plugging equation (5) into (1) it gives:

$$\frac{dm}{dt} = -|k_c|.4 \cdot \pi \cdot \left(\frac{3m}{0.08\pi\rho} \right)^{2/3} \quad (6)$$

$$\frac{dm}{dt} = -|k_c|.4 \cdot \pi \cdot \left(\frac{3}{0.08\pi\rho} \right)^{2/3} m^{2/3} \quad (7)$$

that:

$$A = -|k_c|.4 \cdot \pi \cdot \left(\frac{3}{0.08\pi\rho} \right)^{2/3} \quad (8)$$

$$\frac{dm}{dt} = -A m^{2/3} \quad (9)$$

$$\int_{m_0}^m \frac{dm}{m^{2/3}} = -A \int_0^t dt \quad (10)$$

$$m(t) = m_0 - A m_0^{\frac{2}{3}} t + \frac{1}{3} A^2 m_0^{\frac{1}{3}} t^2 - \frac{1}{27} A^3 t^3 \quad (11)$$

Where $m_0 = m(t=0)$ is the mass of the yet untouched xylose crystal, $m(t)$ is the mass of xylose dissolved at time “ t ”, A is a constant defined according to equation (8) and, t is the time of experiment.

Using equation 11 is possible to correlate the mass variation (proportional to the area of the xylose crystals) with time through the parameter A . This allows estimating the average mass transfer coefficient for each ES system.

References

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