

## Supporting Information

### **The Impact of Sulfur-containing Inorganic Compounds during the Depolymerization of Lignin by Hydrothermal Liquefaction of Black Liquor**

*Maximilian Wörner (maximilian.woerner@kit.edu)\*<sup>†</sup>, Lukas Werner*

*(lukaswerner94@web.de)<sup>†</sup>, Ursel Hornung (ursel.hornung@kit.edu)<sup>†</sup>, Nicholas Islongo*

*Canabarro (nicholas.canabarro@sintef.no)<sup>‡</sup>, David Baudouin (david.baudouin@psi.ch)<sup>‡</sup>,*

*Nicolaus Dahmen (nicolaus.dahmen@kit.edu)<sup>†</sup>*

<sup>†</sup>Karlsruhe Institute of Technology (KIT), Institute of Catalysis Research and Development

(IKFT), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

<sup>‡</sup>Paul-Scherrer-Institute (PSI), Bioenergy and Catalysis Laboratory (LBK), Forschungsstrasse

111, 5232 Villigen, Switzerland

**Table S1.** Weighed-in masses of the compounds and volume of the NaOH/KOH solution for each

model liquor

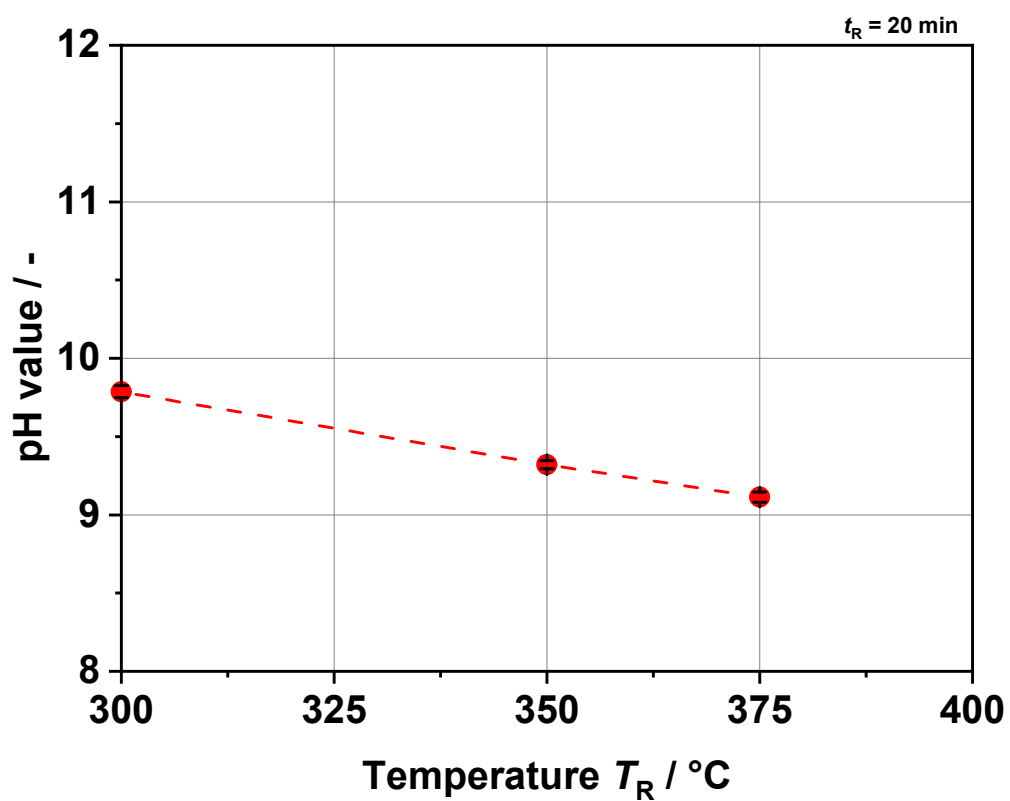
	<b>MBL-A</b>	<b>MBL-B</b>	<b>MBL-C</b>	<b>MBL-D</b>
<b>Na<sub>2</sub>CO<sub>3</sub> / g</b>	1.777	1.778	1.778	1.781
<b>K<sub>2</sub>CO<sub>3</sub> / g</b>	0.183	0.215	0.244	0.275
<b>Na<sub>2</sub>SO<sub>3</sub> / g</b>	0.132	0.133	0.131	0.132
<b>Na<sub>2</sub>SO<sub>4</sub> / g</b>	0.110	0.109	0.106	0.109
<b>Na<sub>2</sub>S<sub>2</sub>O<sub>3</sub> / g</b>	0.195	0.196	0.195	0.194
<b>Na<sub>2</sub>S * 9 H<sub>2</sub>O / g</b>	0	0.785	1.573	2.363
<b>Lignin / g</b>	9.001	8.998	8.998	9.002
<b>NaOH/KOH solution / ml</b>	8.75	7.5	6.25	5
<b>HS<sup>-</sup> / g·l<sup>-1</sup></b>	0	approx. 1	approx. 2	approx. 3

**Table S2.** Volumes of BL used at specific reaction temperatures  $T_R$

$T_R$	250 – 275 °C	300 – 350 °C	375 °C	400 °C
$V_{BL}$	17,5 ml	15 ml	12,5 ml	5 ml

**Table S3.** Distribution coefficients for different catechols when using the described extraction procedure

Component name	Distribution coefficient $K_i$
Catechol	0.82
3-Methylcatechol	0.83
4-Methylcatechol	0.7



**Figure S1.** pH values for the liquid product after HTL of BL at three different reaction temperatures

$T_R$  (300 °C, 350 °C, 375 °C) and holding time  $t_R = 20$  min

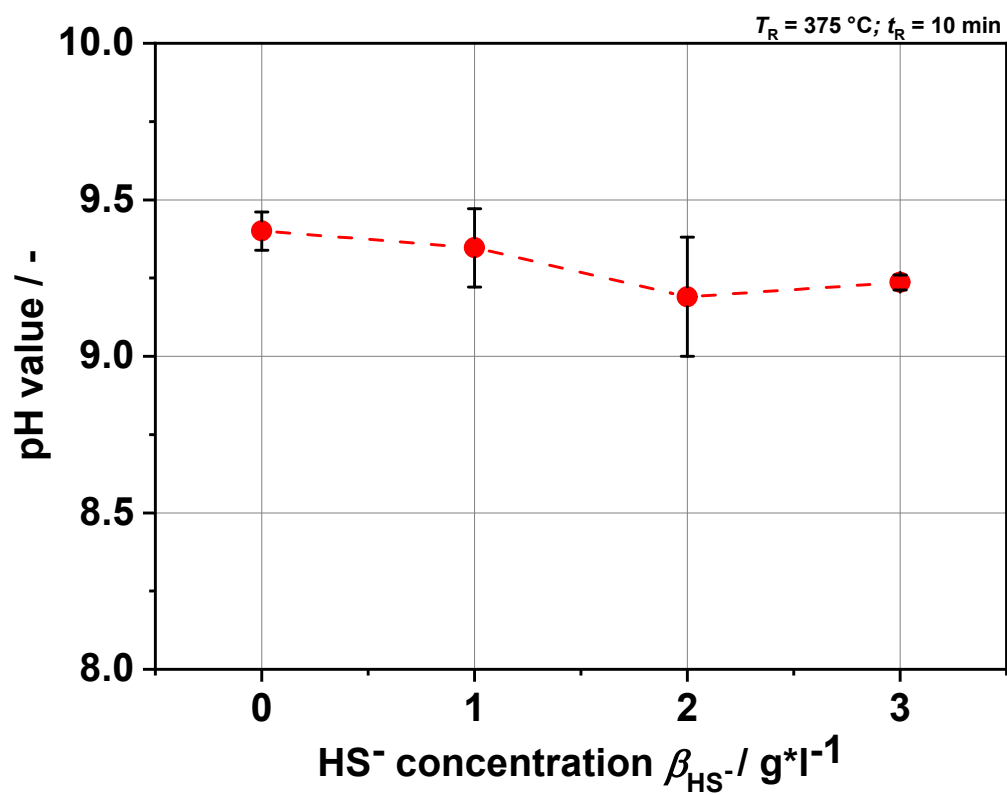


Figure S2. pH values for the liquid product after HTL of MBL at  $T_R = 375 \text{ }^\circ\text{C}$  and  $t_R = 10 \text{ min}$  with different HS<sup>-</sup> feedstock concentrations

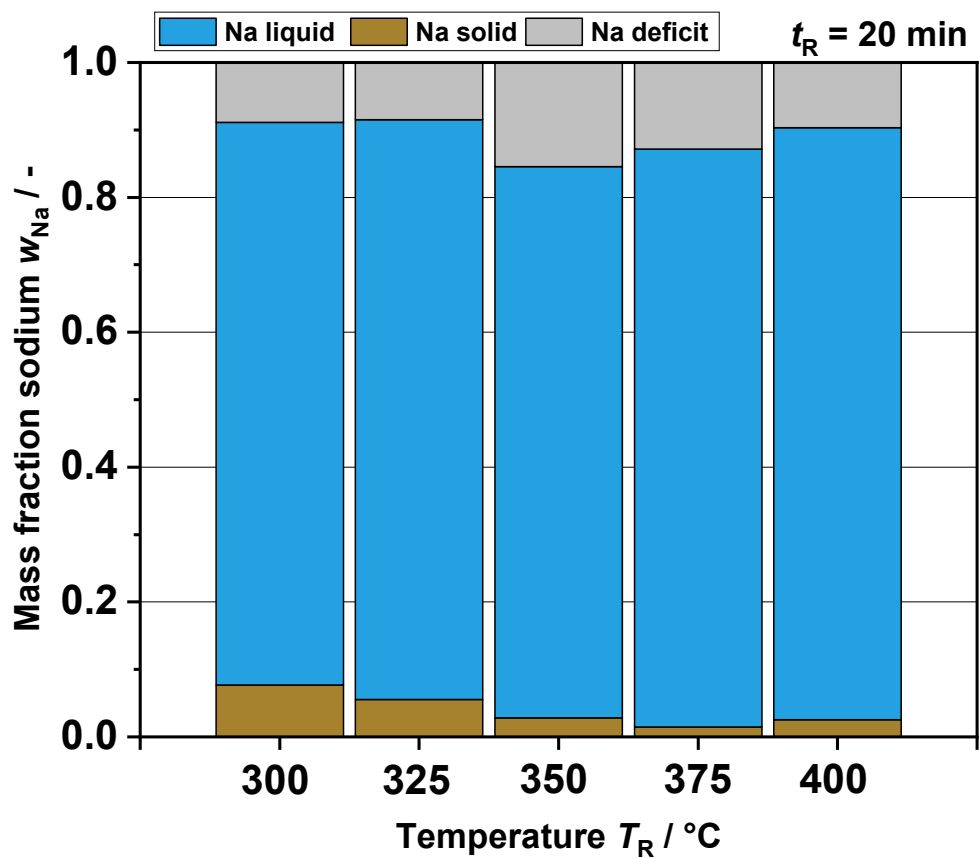


Figure S3. Sodium mass balance at different reaction temperatures  $T_R$

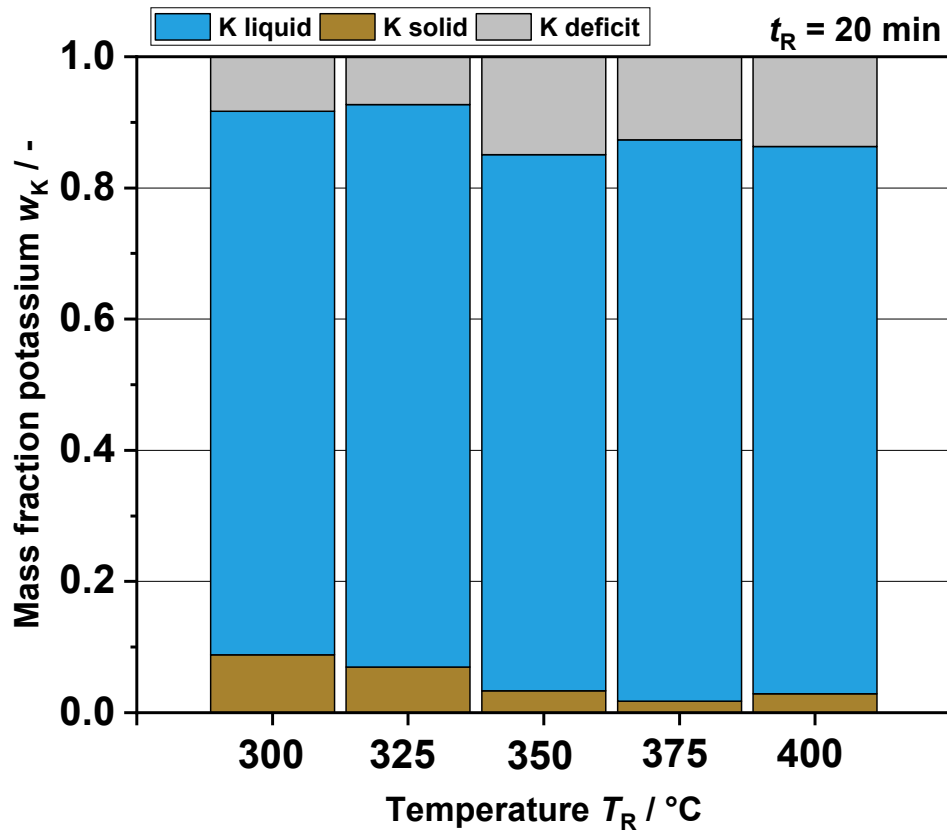


Figure S4. Potassium mass balance at different reaction temperatures  $T_R$