

Supplementary materials

Article

The feasibility of replacing coal with biomass in iron-ore pelletizing plants with respect to melt-induced slagging

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Section A_ Tables

Table S1. Chemical composition and calorimetric analysis of the solid biomasses[1, 2]

	Stem wood	Bark	Forest residue	Willow	Reed canary grass
Proximate analysis					
Water (wt %)	4.3	6.5	3.6	5.9	3.6
Ash (wt %, ds)	0.3	2.0	2.4	1.8	2.4
Ultimate analysis (wt %, ds)					
C	51.3	53.5	51.9	49.6	49.5
H	6.2	6.4	6.2	6.0	6.1
O	42.0	37.7	39.9	42.0	40.4
N	0.1	0.4	0.4	0.5	1.4
Cl	<0.02	<0.02	<0.02	<0.02	0.03
Inorganics (mg kg⁻¹, ds)					
Al	17.41	133.9	309.1	149.8	396.4
Ca	587.5	6197	2666	4603	2795
Fe	3.31	19.66	46.17	31.15	276.2
K	303.0	1444	1494	1610	1685
Mg	105.5	627.2	410.7	335.3	627.2
Mn	64.98	446.1	242.4	17.27	240.1
Na	23.22	118.7	112.8	109.8	79.38
P	25.66	358.7	312.5	467.0	1510
S	211.0	294.0	236.0	412.0	1340
Si	67.31	148.2	1262.	724.5	4062
Ti	0.60	2.34	13.31	7.37	11.87
Zn	8.73	123.0	48.90	54.70	61.20
Calorimetric analysis					
(MJ kg ⁻¹ , ds)					
Effective heating value	19.3	20.7	19.6	18.4	18.6

Table S2. Chemical composition and calorimetric analysis of the pyrolysis oils (PO)[1, 2]

	Stem wood	Bark	Forest residue	Willow	Reed canary grass
Proximate analysis					
Water (wt %)	17.7	24.8	20.7	20.3	17.5
Ash (wt %, ds)	<0.01	0.04	0.03	0.05	0.04
Ultimate analysis (wt %, ds)					
C	56.0	55.9	56.2	55.0	55.6
H	6.4	7.4	6.1	6.5	6.7
O	37.5	36.3	37.3	38.2	36.3
N	<0.1	0.3	0.4	0.3	1.4
Cl	0.009	-	-	-	-
Inorganics (mg kg⁻¹, ds)					
Al	0.77	<0.9	1.81	0.95	3.99
Ca	8.85	<11	17.44	37.92	42.98
Fe	1.25	1.56	2.85	2.53	12.13
K	13.49	23.27	51.57	63.63	45.59
Mg	<1.5	1.18	2.94	2.75	13.17
Mn	0.75	0.84	1.83	0.22	4.69
Na	<3	1.28	<3	<3	<4
P	2.90	2.92	5.50	7.23	33.43
S	116.4	122.4	125.7	157.3	790.3
Si	1.57	<9	2.53	2.31	11.07
Ti	<0.1	<0.5	<0.1	<0.1	0.153
Zn	1.51	5.09	3.65	2.86	4.02
Calorimetric analysis					
(MJ kg⁻¹, ds)					
Effective heating value	21.7	23.6	22.4	21.0	21.3

Table S3. Chemical composition and calorimetric analysis of the biochar[1, 2]

	Stem wood	Bark	Forest residue	Willow	Reed canary grass
Proximate analysis					
Water (wt %)	-	-	-	-	-
Ash (wt %, ds)	2.1	9.0	9.5	12.8	14.2
Ultimate analysis (wt %, ds)					
C	67.8	71.6	72.9	70.1	68.4
H	4.9	3.7	3.3	3.3	2.9
O	24.9	14.8	13.4	12.6	11.9
N	0.25	0.69	0.74	1.01	2.35
Cl	<0.02	<0.02	0.03	0.06	0.04
Inorganics (mg kg⁻¹, ds)					
Al	116.4	608.6	1683	730.4	725.1
Ca	4939	29020	20080	34160	16150
Fe	21.16	81.08	249.6	218.5	691.5
K	2341	7247	11950	12540	12700
Mg	892.5	2883	3160	2653	5204
Mn	563.8	2052	1928	123.1	1750
Na	204.0	514.9	626.1	656.5	257.4
P	214.3	1658	2483	3683	9339
S	243.0	236.0	248.0	1050	1290
Si	385.6	626.4	6077	3552	21740
Ti	3.78	9.95	67.75	31.59	30.87
Zn	50.50	562.0	317.0	394.0	458.0
Calorimetric analysis					
(MJ kg⁻¹, ds)					
Effective heating value	26.0	26.1	26.5	25.2	25.1

Table S4. The chemical composition of the coal and pellet-dust used in the TECs

Coal/Pellet-dust	Coal	Pellet-dust
Proximate analysis (wt.% as received)		
Volatile matter	21.2	-
Fixed carbon	62.2	-
Moisture	4.2	11.2
Ash content (coals)/minerals (pellet-dust)	12.4	88.8
Ultimate analysis (wt.% dry)		
C	76.4	-
H	4.0	-
N	1.39	-
O	5.1	30.60
Cl	0.01	<0.002
S	0.323	<0.001
Lower heating value (MJ/kg dry)	30.4	-
Major inorganic elements (wt.% dry fuel)		
Si	3.27	0.98
Al	2.09	0.12
Ca	0.22	0.33
Fe	0.40	66.91
K	0.07	0.03
Mg	0.05	0.90
Mn	0.00	0.06
Na	0.04	0.03
P	0.08	0.025
Ti	0.09	0.09

Table S5. List of the phases used in the equilibrium calculations in the system SiO₂-Al₂O₃-CaO-MgO-FeO-Fe₂O₃-Na₂O-K₂O

Name	Model	Composition/formula	Comments
oxide melt (slag)	modified associate species model Multi sub-lattice model using Compound Energy Formalism	basic oxides + binary and ternary liquid species	+ all interactions between them
(K,Na)(Fe,Al)O ₂ _HT		(Al ³⁺ ,Si ⁴⁺ ,Fe ³⁺) ₁ (Na ¹⁺ ,K ¹⁺ ,Va) ₁ (O ²⁻) ₂	high T phase Alk(Al, Fe)O ₂
(K,Na)(Fe,Al)O ₂ _LT		Al ³⁺ ,Si ⁴⁺ ,Fe ³⁺) ₁ (Na ¹⁺ ,K ¹⁺ ,Va) ₁ (O ²⁻) ₂	high T phase Alk(Al, Fe)O ₂
Corundum		(Al ³⁺ ,Fe ³⁺) ₂ (O ²⁻) ₃	Me ₂ O ₃ phase
KAF4S3		(Al ³⁺ ,Fe ³⁺) ₄ (K ¹⁺) ₄ (Si ⁴⁺) ₃ (O ²⁻) ₁₄	(K,Na) ₄ Al ₄ Si ₃ O ₁₄ phase
Kaliophilite-HT		(Al ³⁺ ,Fe ³⁺) ₂ (K ¹⁺ , Na ¹⁺) ₂ (Si ⁴⁺) ₂ (O ²⁻) ₈	HT phase KFeSiO ₄ -KAlSiO ₄
Kaliophilite-LT		(Al ³⁺ ,Fe ³⁺) ₂ (K ¹⁺ , Na ¹⁺) ₂ (Si ⁴⁺) ₂ (O ²⁻) ₈	LT phase KFeSiO ₄ -KAlSiO ₄
Leucite		(Al ³⁺ ,Fe ³⁺) ₂ (K ¹⁺) ₂ (Si ⁴⁺) ₄ (O ²⁻) ₁₂	Quaternary phase KFeSi ₂ O ₆ -KAlSi ₂ O ₆
Nepheline		(Al ³⁺ ,Si ⁴⁺) ₂ (Va) ₁ (Na ¹⁺ ,K ¹⁺ ,Va) ₁ (O ²⁻) ₄	(Na,K)AlSiO ₄ -LT
Carnegieite		(Al ³⁺ ,Si ⁴⁺) ₂ (Va) ₁ (Na ¹⁺ ,K ¹⁺ ,Va) ₁ (O ²⁻) ₄	(Na,K)AlSiO ₄ -HT
Fe ₁₂ K ₂ O ₁₉ _S1	Stoichiometric compounds	Fe ₁₂ K ₂ O ₁₉	-

References

1. Johansson, A.-C., et al., *Characterization of pyrolysis products produced from different Nordic biomass types in a cyclone pilot plant*. Fuel processing technology, 2016. **146**: p. 9-19.
2. Winikka, H., et al., *Fate of inorganic elements during fast pyrolysis of biomass in a cyclone reactor*. Fuel, 2017. **203**: p. 537-547.

Section B_ Plots for the investigated raw biomasses

Description of the different plots:

1- Slag frac. & visc.: Mass fraction of the molten slag (melt) in the condensed phases predicted for the raw biomasses, together with the estimated viscosity of the respective molten slag. Color shading refers to the mass fraction of the predicted melt (slag fraction) and the iso-viscosity lines (contours) refer to the estimated viscosities of the respective melt fractions in Pa.s.

2- QSI: Calculated QSI values [where $QSI = \ln(1/\mu)$, and μ is the viscosity of the molten fraction of the condensed phases] for the raw biomasses. Color shading refers to the calculated QSI.

3- B/A ratio: Calculated B/A absolute values as the ratio of network modifiers/ network formers for the raw biomasses. Color shading refers to the calculated absolute values (B/A).

The following equation is the ratio of “network modifiers” to “network formers”:

$$\frac{B}{A} = \frac{\text{Network modifiers}}{\text{Network formers}} = \frac{CaO + MgO + K_2O + Na_2O + Fe_2O_3 + FeO}{SiO_2 + Al_2O_3}$$

where SiO_2 , etc., represent the mole fractions predicted for the major components in the respective predicted molten slags of the investigated fuels.

4- ADT: Plots of absolute deposition tendency (as defined in the manuscript) calculated for the raw biomasses.

5- Δ Slag frac. & visc.: Δ (slag frac.) values calculated for the TEC results of the raw biomasses under the definition, $\Delta(\text{slag frac.}) = (\text{slag frac.})_{\text{raw biomass}} - (\text{slag frac.})_{\text{ref}}$, where $(\text{slag frac.})_{\text{raw biomass}}$ and $(\text{slag frac.})_{\text{ref}}$ are mass fractions of the molten slag (melt) in the condensed phases calculated for the raw biomasses and the reference case (either coal or stem wood), respectively. The melt fractions predicted for the raw biomasses are less than the reference case (either coal or stem wood) if $\Delta(\text{slag frac.}) < 0$, and higher if $\Delta(\text{slag frac.}) > 0$. Color shading refers to the calculated Δ Slag frac.

6- Δ QSI: $\Delta(QSI)$ values calculated for the TEC results of the raw biomasses under the definition, $\Delta(QSI) = (QSI)_{\text{raw biomass}} - (QSI)_{\text{ref}}$, where $(QSI)_{\text{raw biomass}}$ and $(QSI)_{\text{ref}}$ are the calculated QSI values for the raw biomasses and the reference case (either coal or stem wood), respectively. The QSI calculated for the raw biomasses are less than the reference case (either coal or stem wood) if $\Delta(QSI) < 0$, and higher if $\Delta(QSI) > 0$. Color shading refers to the calculated Δ QSI.

7- Δ B/A: $\Delta(B/A)$ values calculated for the TEC results of the raw biomasses under the definition, $\Delta(B/A) = (B/A)_{\text{raw biomass}} - (B/A)_{\text{ref}}$, where $(B/A)_{\text{raw biomass}}$ and $(B/A)_{\text{ref}}$ are the calculated B/A ratios for the raw biomasses and the reference case (either coal or stem wood), respectively. The B/A calculated for the raw biomasses are less than the reference case (either coal or stem wood) if $\Delta(B/A) < 0$, and higher if $\Delta(B/A) > 0$. Color shading refers to the calculated Δ B/A.

8- Δ ADT: $\Delta(ADT)$ values calculated for the TEC results of the raw biomasses under the definition, $\Delta(ADT) = (ADT)_{\text{raw biomass}} - (ADT)_{\text{ref}}$, where $(ADT)_{\text{raw biomass}}$ and $(ADT)_{\text{ref}}$ are the calculated ADTs for the raw biomasses and the reference case (either coal or stem wood), respectively. The ADT calculated for the raw biomasses are less than the reference case (either coal or stem wood) if $\Delta(ADT) < 0$, and higher if $\Delta(ADT) > 0$. Color shading refers to the calculated Δ ADT.

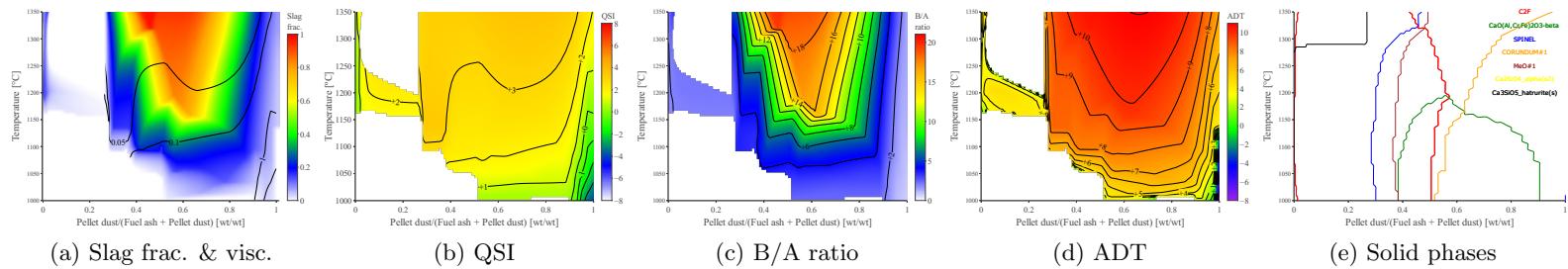


Figure S1: Bark absolute plots

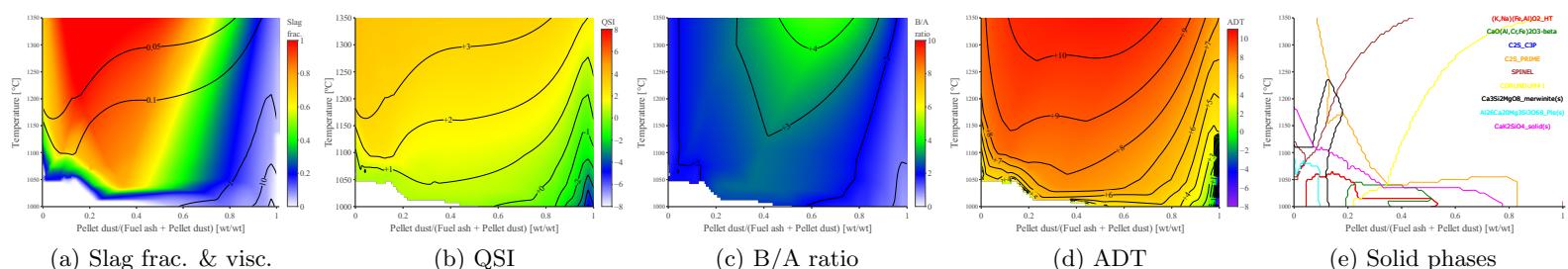


Figure S2: Forest residue absolute plots

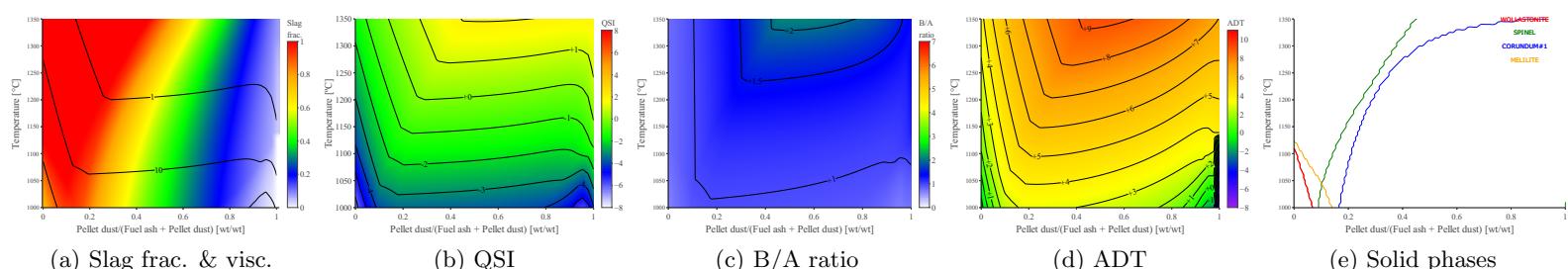


Figure S3: Reed-Canary-grass absolute plots

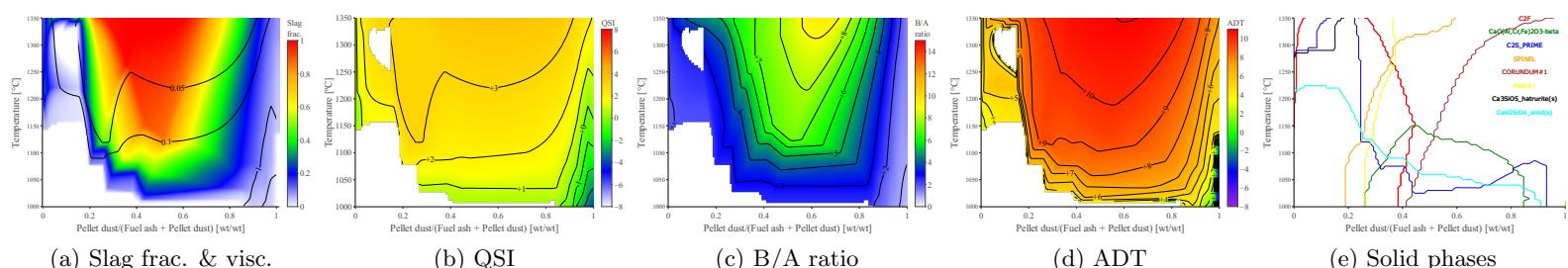


Figure S4: Willow absolute plots

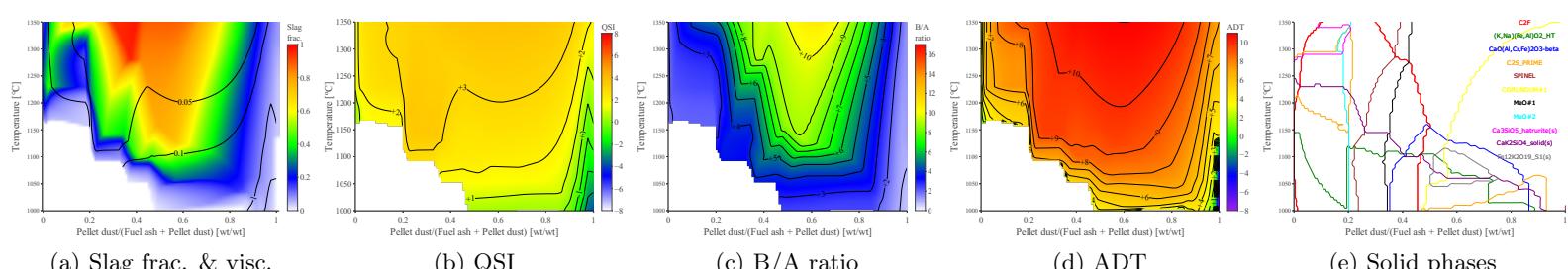


Figure S5: Stemwood absolute plots

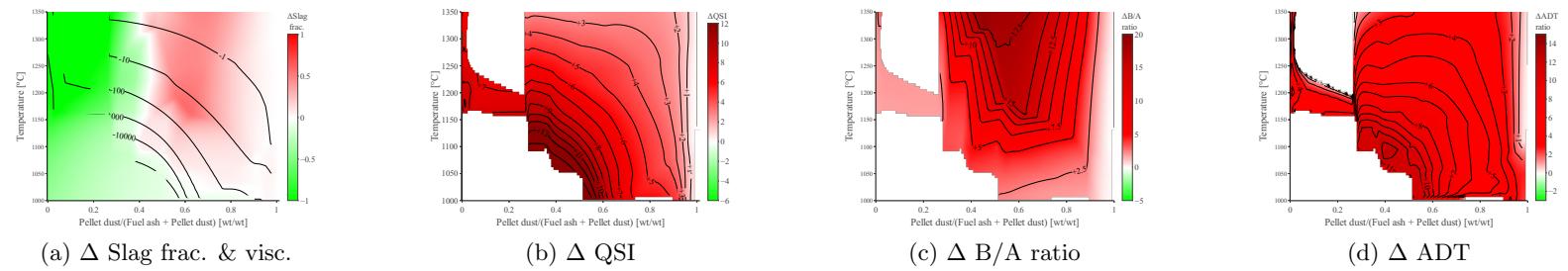


Figure S6: Bark difference (coal reference) plots

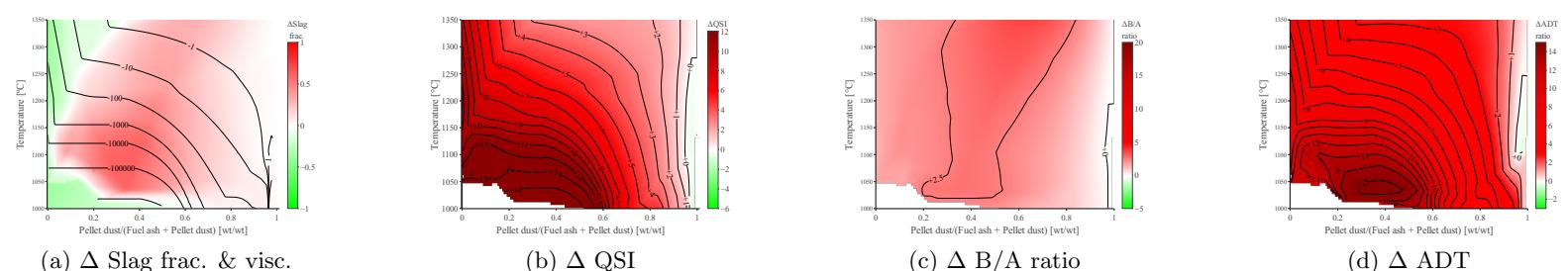


Figure S7: Forest residue difference (coal reference) plots

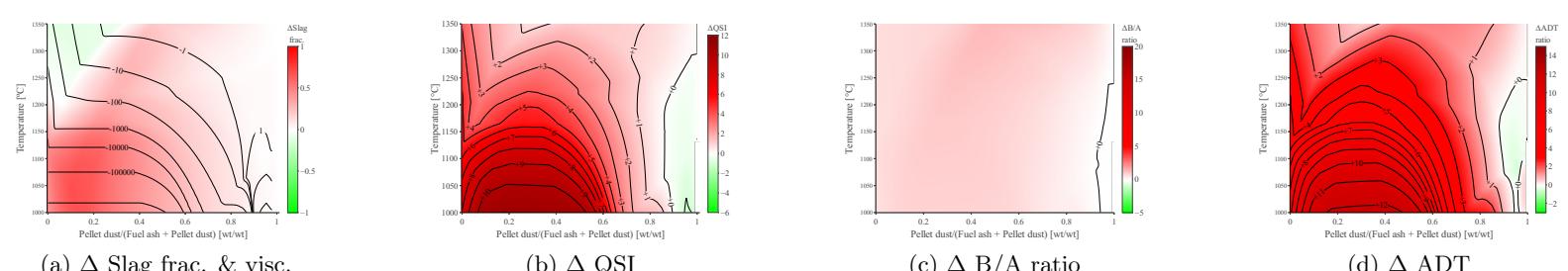


Figure S8: Reed-Canary-grass difference (coal reference) plots

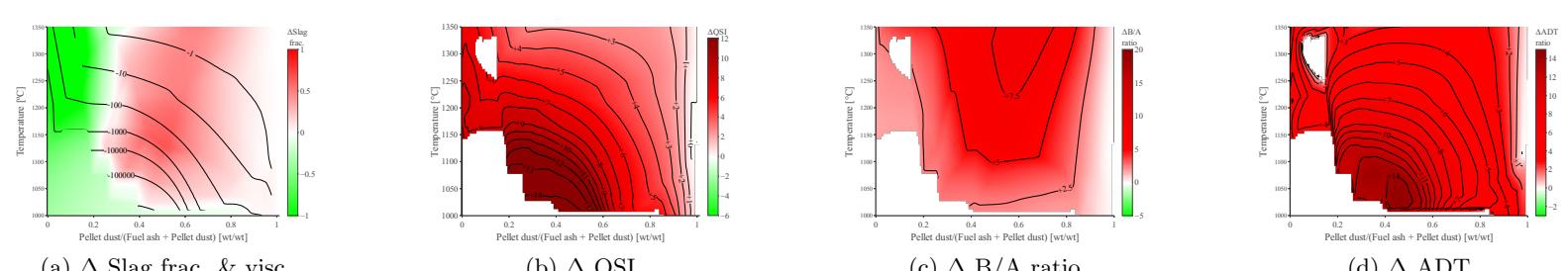


Figure S9: Willow difference (coal reference) plots

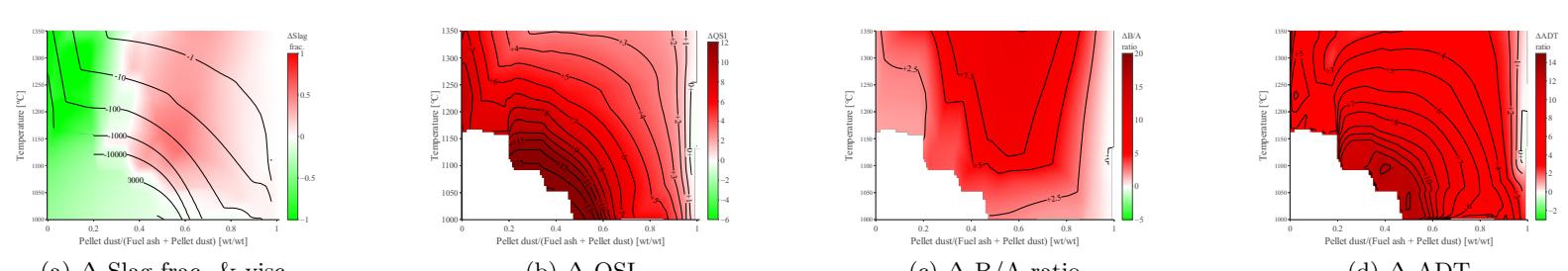


Figure S10: Stemwood difference (coal reference) plots

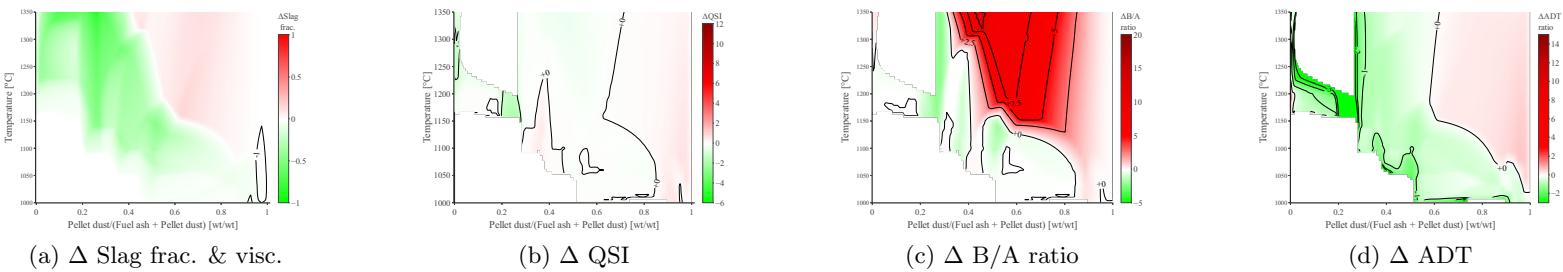


Figure S11: Bark difference (Solid-Biomass stemwood reference) plots

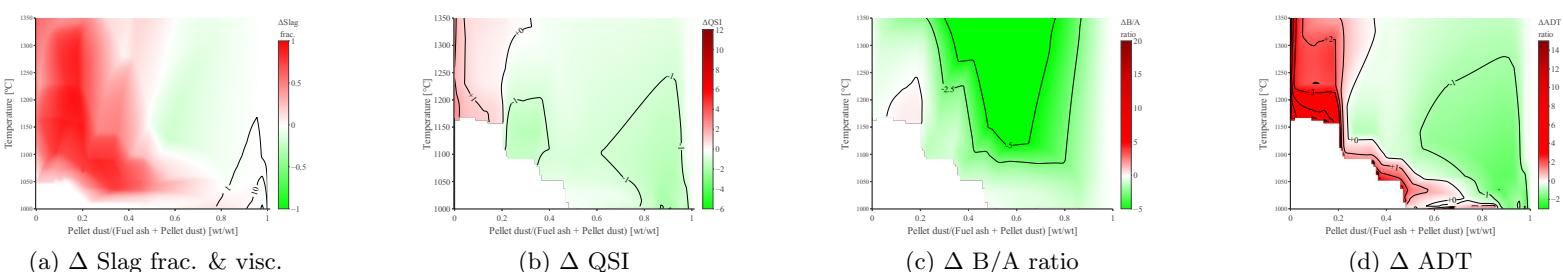


Figure S12: Forest residue difference (Solid-Biomass stemwood reference) plots

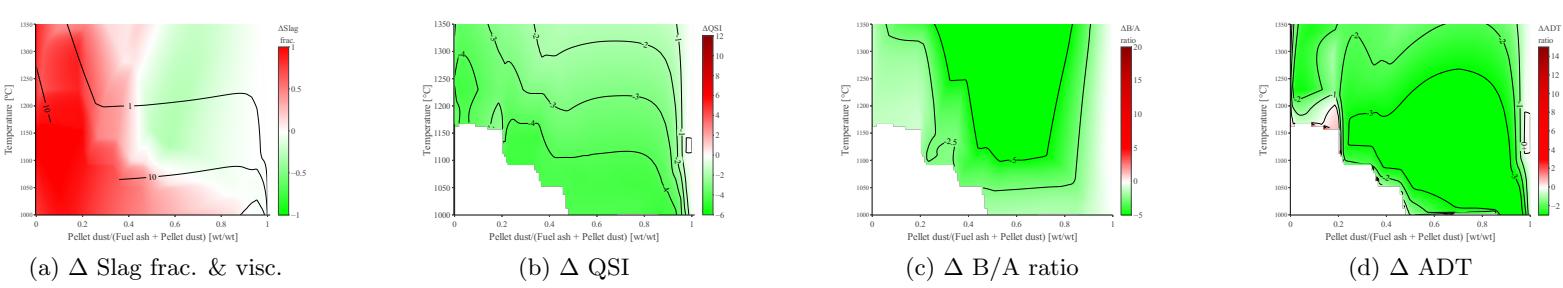


Figure S13: Reed-Canary-grass difference (Solid-Biomass stemwood reference) plots

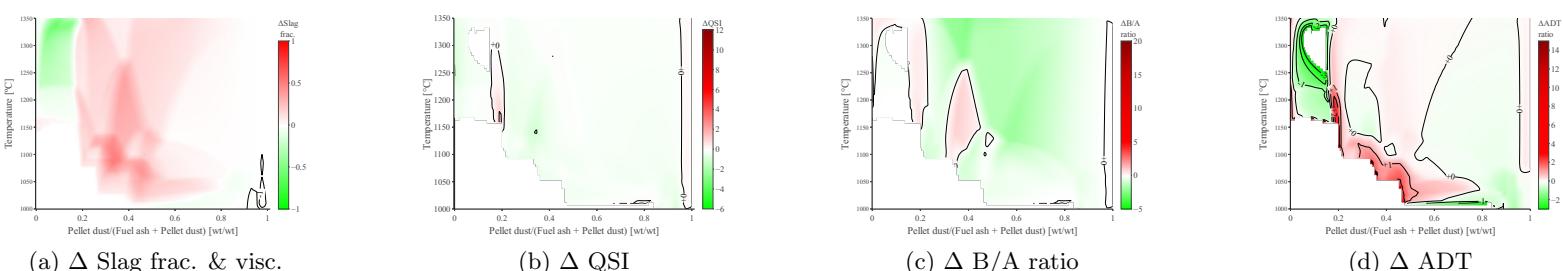


Figure S14: Willow difference (Solid-Biomass stemwood reference) plots

Section C_ Plots for the investigated pyrolysis oils (bio-oil)

Description of the different plots:

1- Slag frac. & visc.: Mass fraction of the molten slag (melt) in the condensed phases predicted for the pyrolysis oils (PO), together with the estimated viscosity of the respective molten slag. Color shading refers to the mass fraction of the predicted melt (slag fraction) and the iso-viscosity lines (contours) refer to the estimated viscosities of the respective melt fractions in Pa.s.

2- QSI: Calculated QSI values [where $QSI = \ln(1/\mu)$, and μ is the viscosity of the molten fraction of the condensed phases] for the pyrolysis oils. Color shading refers to the calculated QSI.

3- B/A ratio: Calculated B/A absolute values as the ratio of network modifiers/ network formers for the pyrolysis oils. Color shading refers to the calculated absolute values (B/A).
The following equation is the ratio of “network modifiers” to “network formers”:

$$\frac{B}{A} = \frac{\text{Network modifiers}}{\text{Network formers}} = \frac{CaO + MgO + K_2O + Na_2O + Fe_2O_3 + FeO}{SiO_2 + Al_2O_3}$$

where SiO_2 , etc., represent the mole fractions predicted for the major components in the respective predicted molten slags of the investigated fuels.

4- ADT: Plots of absolute deposition tendency (as defined in the manuscript) calculated for the pyrolysis oils.

5- Δ Slag frac. & visc.: $\Delta(\text{slag frac.})$ values calculated for the TEC results of the pyrolysis oils under the definition, $\Delta(\text{slag frac.}) = (\text{slag frac.})_{\text{PO}} - (\text{slag frac.})_{\text{ref}}$, where $(\text{slag frac.})_{\text{PO}}$ and $(\text{slag frac.})_{\text{ref}}$ are mass fractions of the molten slag (melt) in the condensed phases calculated for the pyrolysis oils and the reference case (either coal or stem wood-PO), respectively. The melt fractions predicted for the pyrolysis oils are less than the reference case (either coal or stem wood-PO) if $\Delta(\text{slag frac.}) < 0$, and higher if $\Delta(\text{slag frac.}) > 0$. Color shading refers to the calculated Δ Slag frac.

6- Δ QSI: $\Delta(QSI)$ values calculated for the TEC results of the pyrolysis oils under the definition, $\Delta(QSI) = (QSI)_{\text{PO}} - (QSI)_{\text{ref}}$, where $(QSI)_{\text{PO}}$ and $(QSI)_{\text{ref}}$ are the calculated QSI values for the pyrolysis oils and the reference case (either coal or stem wood-PO), respectively. The QSI calculated for the pyrolysis oils are less than the reference case (either coal or stem wood-PO) if $\Delta(QSI) < 0$, and higher if $\Delta(QSI) > 0$. Color shading refers to the calculated Δ QSI.

7- Δ B/A: $\Delta(B/A)$ values calculated for the TEC results of the pyrolysis oils under the definition, $\Delta(B/A) = (B/A)_{\text{PO}} - (B/A)_{\text{ref}}$, where $(B/A)_{\text{PO}}$ and $(B/A)_{\text{ref}}$ are the calculated B/A ratios for the pyrolysis oils and the reference case (either coal or stem wood-PO), respectively. The B/A calculated for the pyrolysis oils are less than the reference case (either coal or stem wood-PO) if $\Delta(B/A) < 0$, and higher if $\Delta(B/A) > 0$. Color shading refers to the calculated Δ B/A.

8- Δ ADT: $\Delta(ADT)$ values calculated for the TEC results of the pyrolysis oils under the definition, $\Delta(ADT) = (ADT)_{\text{PO}} - (ADT)_{\text{ref}}$, where $(ADT)_{\text{PO}}$ and $(ADT)_{\text{ref}}$ are the calculated ADTs for the pyrolysis oils and the reference case (either coal or stem wood-PO), respectively. The ADT calculated for the pyrolysis oils are less than the reference case (either coal or stem wood-PO) if $\Delta(ADT) < 0$, and higher if $\Delta(ADT) > 0$. Color shading refers to the calculated Δ ADT.

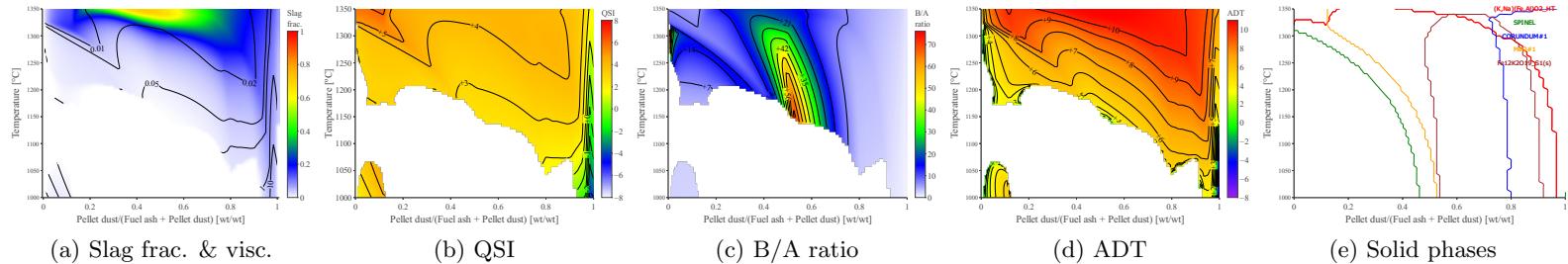


Figure S15: Bark absolute plots

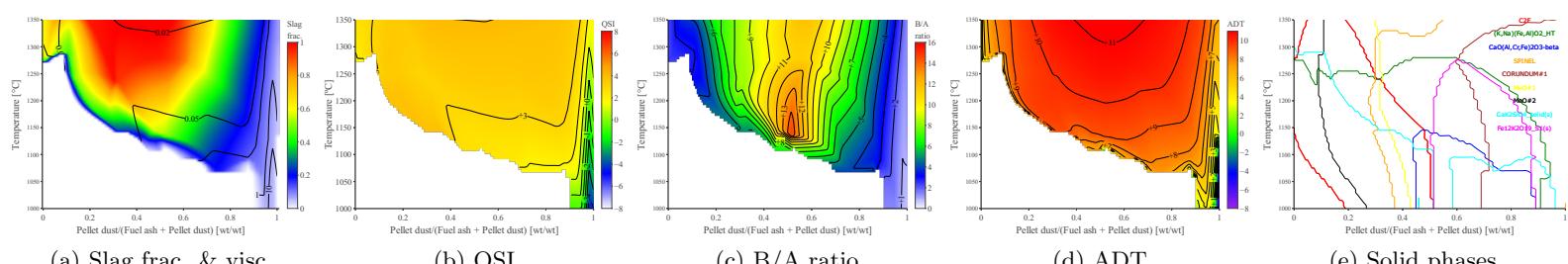


Figure S16: Forest residue absolute plots

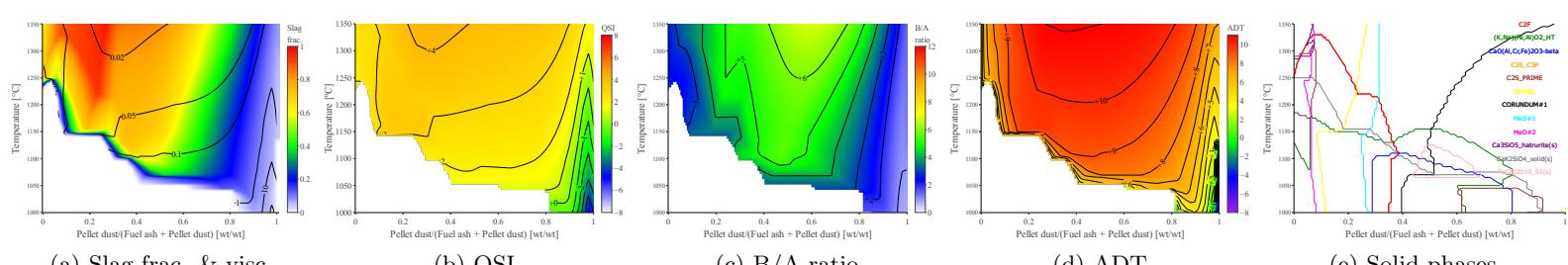


Figure S17: Reed-Canary-grass absolute plots

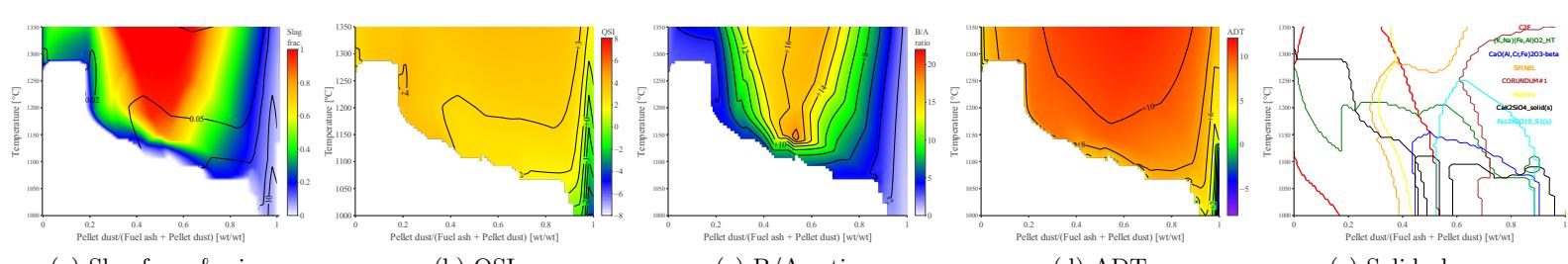


Figure S18: Willow absolute plots

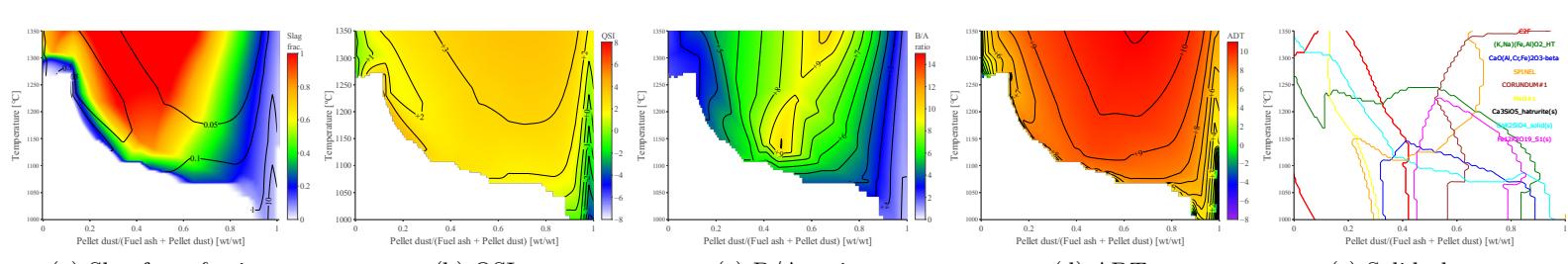


Figure S19: Stemwood absolute plots

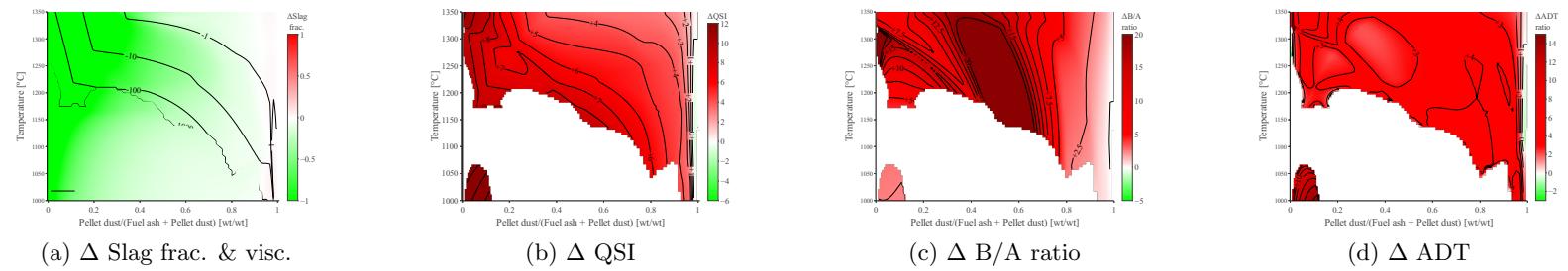


Figure S20: Bark difference (coal reference) plots

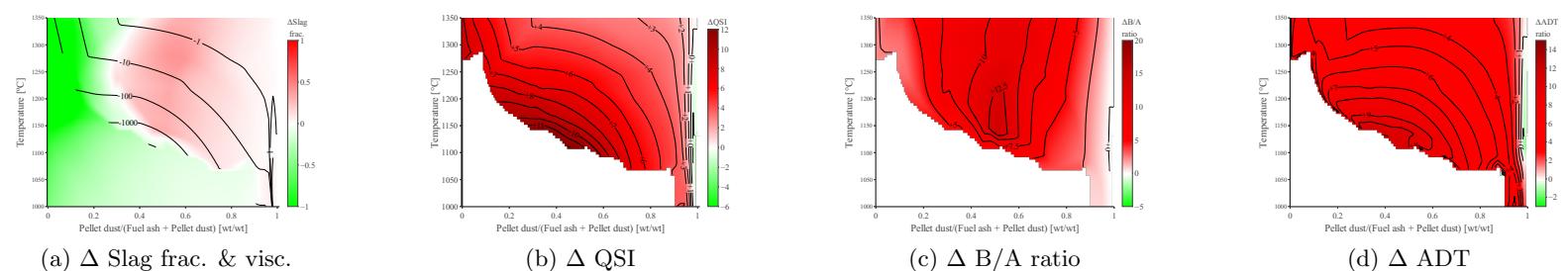


Figure S21: Forest residue difference (coal reference) plots

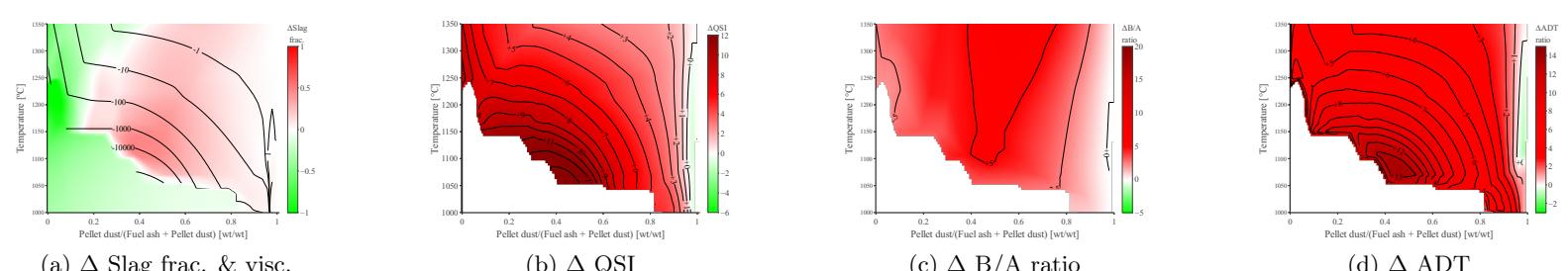


Figure S22: Reed-Canary-grass difference (coal reference) plots

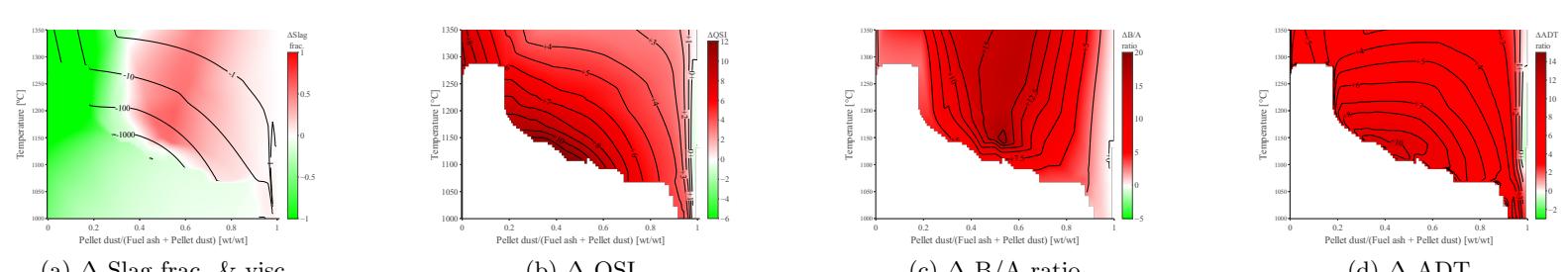


Figure S23: Willow difference (coal reference) plots

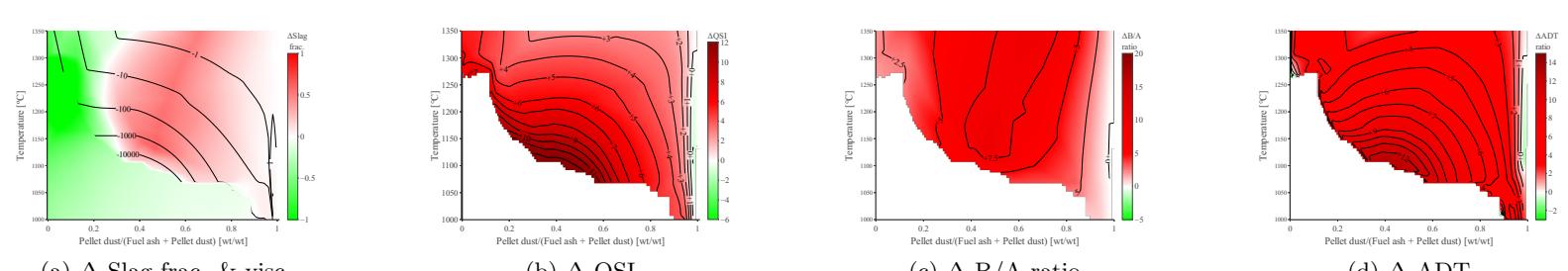


Figure S24: Stemwood difference (coal reference) plots

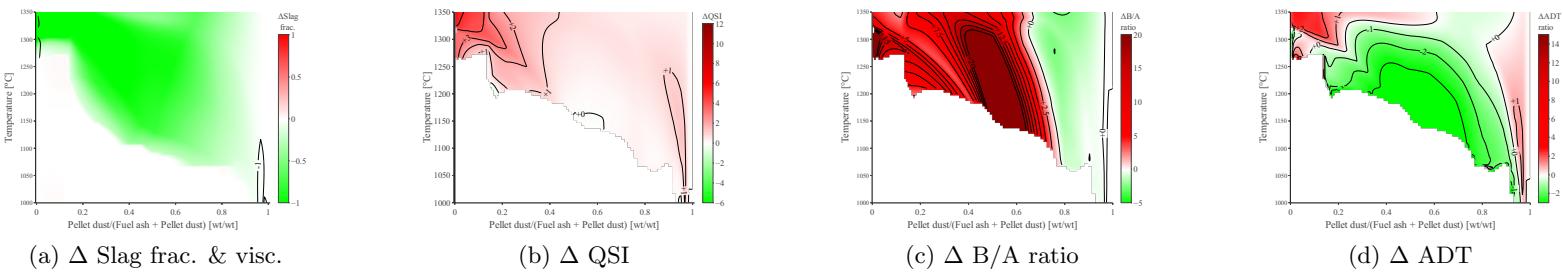


Figure S25: Bark difference (PO stemwood reference) plots

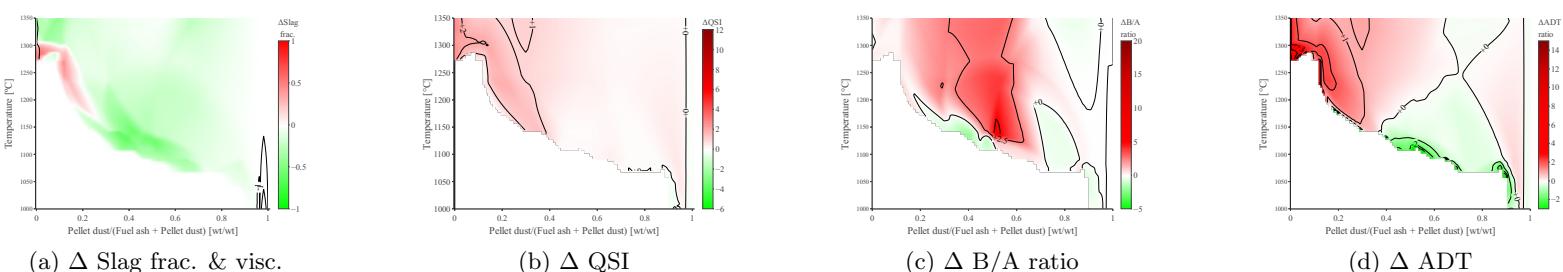


Figure S26: Forest residue difference (PO stemwood reference) plots

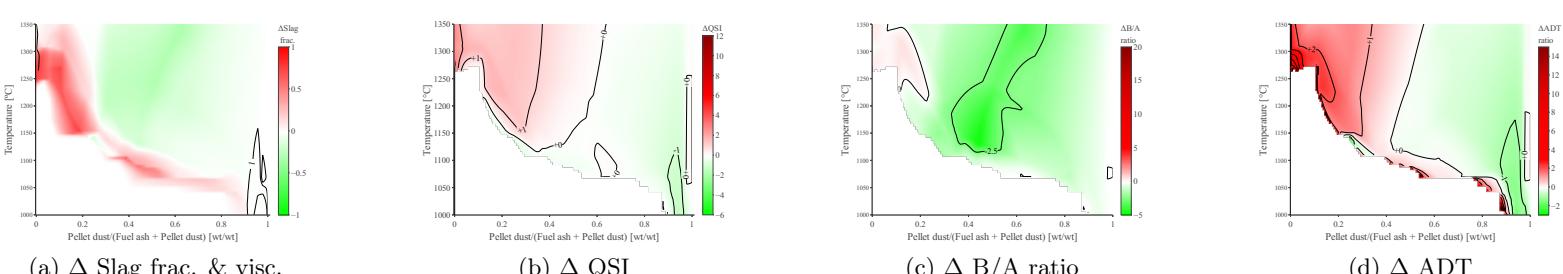


Figure S27: Reed-Canary-grass difference (PO stemwood reference) plots

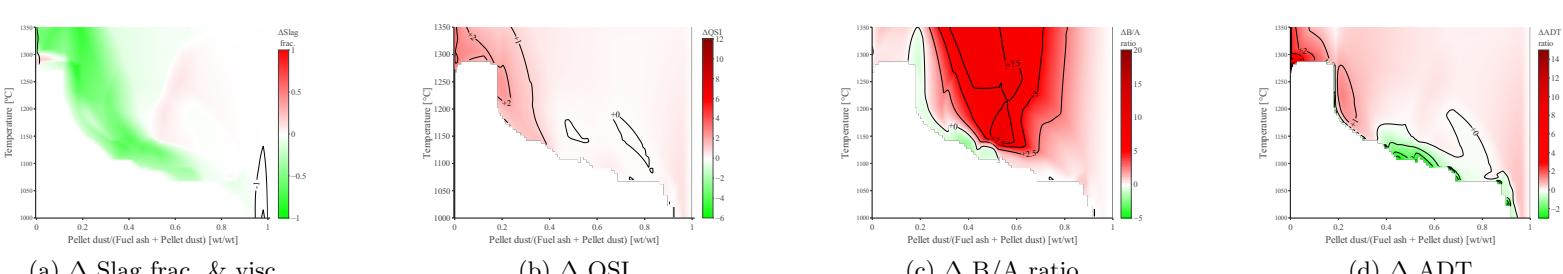


Figure S28: Willow difference (PO stemwood reference) plots

Section D_ Plots for the investigated biochars

Description of the different plots:

1- Slag frac. & visc.: Mass fraction of the molten slag (melt) in the condensed phases predicted for the biochars (BC), together with the estimated viscosity of the respective molten slag. Color shading refers to the mass fraction of the predicted melt (slag fraction) and the iso-viscosity lines (contours) refer to the estimated viscosities of the respective melt fractions in Pa.s.

2- QSI: Calculated QSI values [where $QSI = \ln(1/\mu)$, and μ is the viscosity of the molten fraction of the condensed phases] for the biochars. Color shading refers to the calculated QSI.

3- B/A ratio: Calculated B/A absolute values as the ratio of network modifiers/ network formers for the biochars. Color shading refers to the calculated absolute values (B/A).

The following equation is the ratio of “network modifiers” to “network formers”:

$$\frac{B}{A} = \frac{\text{Network modifiers}}{\text{Network formers}} = \frac{CaO + MgO + K_2O + Na_2O + Fe_2O_3 + FeO}{SiO_2 + Al_2O_3}$$

where SiO_2 , etc., represent the mole fractions predicted for the major components in the respective predicted molten slags of the investigated fuels.

4- ADT: Plots of absolute deposition tendency (as defined in the manuscript) calculated for the biochars.

5- Δ Slag frac. & visc.: Δ (slag frac.) values calculated for the TEC results of the biochars under the definition, $\Delta(\text{slag frac.}) = (\text{slag frac.})_{BC} - (\text{slag frac.})_{ref}$, where $(\text{slag frac.})_{BC}$ and $(\text{slag frac.})_{ref}$ are mass fractions of the molten slag (melt) in the condensed phases calculated for the biochars and the reference case (either coal or stem wood-biochar), respectively. The melt fractions predicted for the biochars are less than the reference case (either coal or stem wood-biochar) if $\Delta(\text{slag frac.}) < 0$, and higher if $\Delta(\text{slag frac.}) > 0$. Color shading refers to the calculated Δ Slag frac.

6- Δ QSI: $\Delta(QSI)$ values calculated for the TEC results of the biochars under the definition, $\Delta(QSI) = (QSI)_{BC} - (QSI)_{ref}$, where $(QSI)_{BC}$ and $(QSI)_{ref}$ are the calculated QSI values for the biochars and the reference case (either coal or stem wood-biochar), respectively. The QSI calculated for the biochars are less than the reference case (either coal or stem wood-biochar) if $\Delta(QSI) < 0$, and higher if $\Delta(QSI) > 0$. Color shading refers to the calculated Δ QSI.

7- Δ B/A: $\Delta(B/A)$ values calculated for the TEC results of the biochars under the definition, $\Delta(B/A) = (B/A)_{BC} - (B/A)_{ref}$, where $(B/A)_{BC}$ and $(B/A)_{ref}$ are the calculated B/A ratios for the biochars and the reference case (either coal or stem wood-biochar), respectively. The B/A calculated for the biochars are less than the reference case (either coal or stem wood-biochar) if $\Delta(B/A) < 0$, and higher if $\Delta(B/A) > 0$. Color shading refers to the calculated Δ B/A.

8- Δ ADT: $\Delta(ADT)$ values calculated for the TEC results of the biochars under the definition, $\Delta(ADT) = (ADT)_{BC} - (ADT)_{ref}$, where $(ADT)_{BC}$ and $(ADT)_{ref}$ are the calculated ADTs for the biochars and the reference case (either coal or stem wood-biochar), respectively. The ADT calculated for the biochars are less than the reference case (either coal or stem wood-biochar) if $\Delta(ADT) < 0$, and higher if $\Delta(ADT) > 0$. Color shading refers to the calculated Δ ADT.

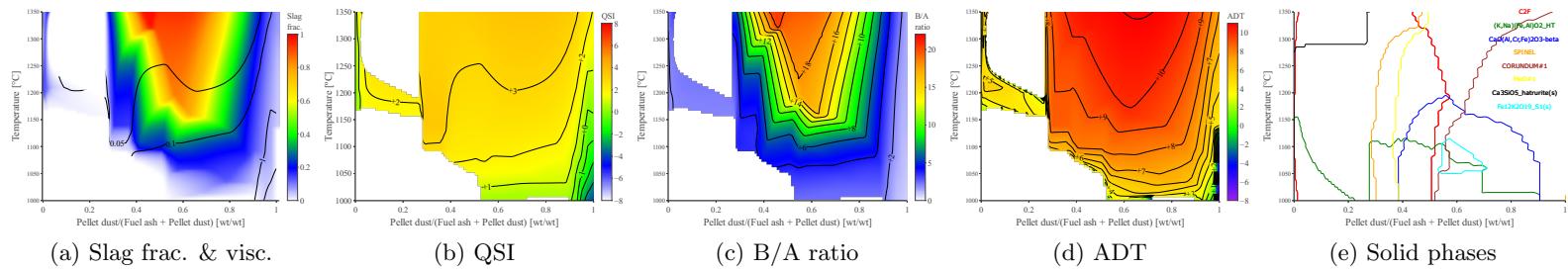


Figure S29: Bark absolute plots

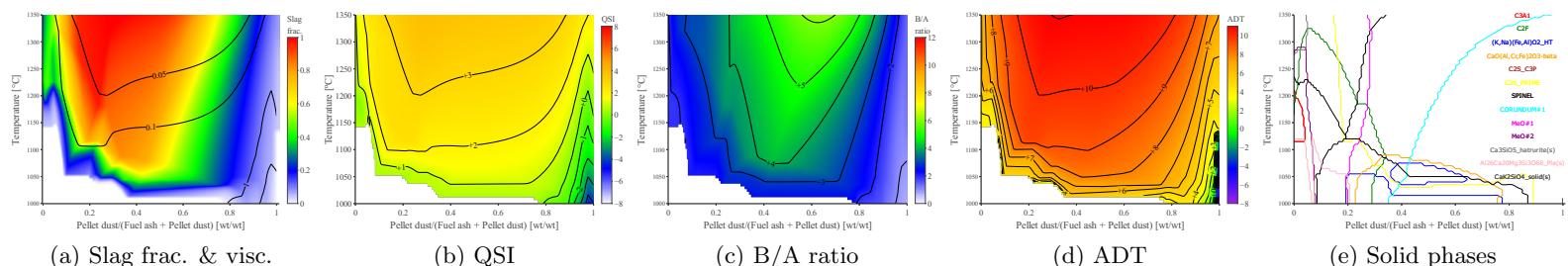


Figure S30: Forest residue absolute plots

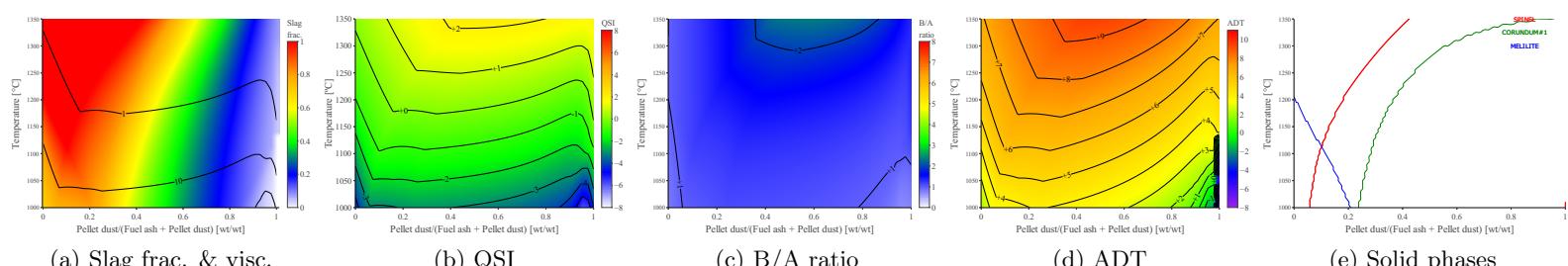


Figure S31: Reed-Canary-grass absolute plots

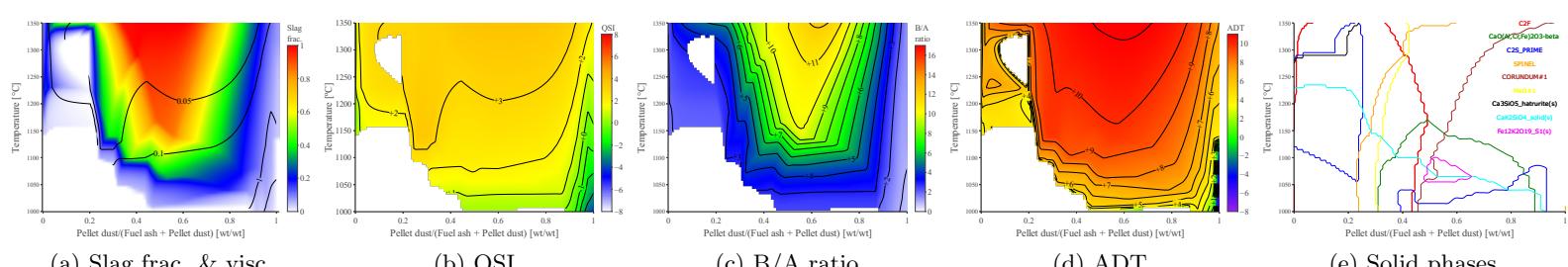


Figure S32: Willow absolute plots

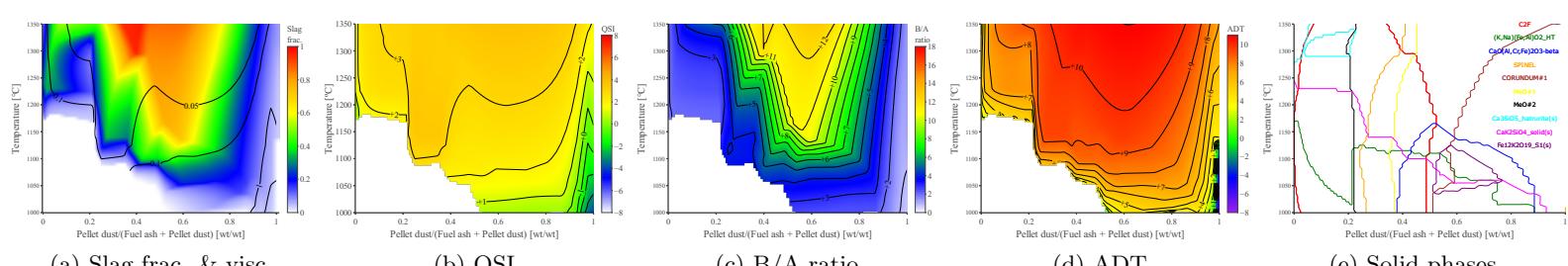


Figure S33: Stemwood absolute plots

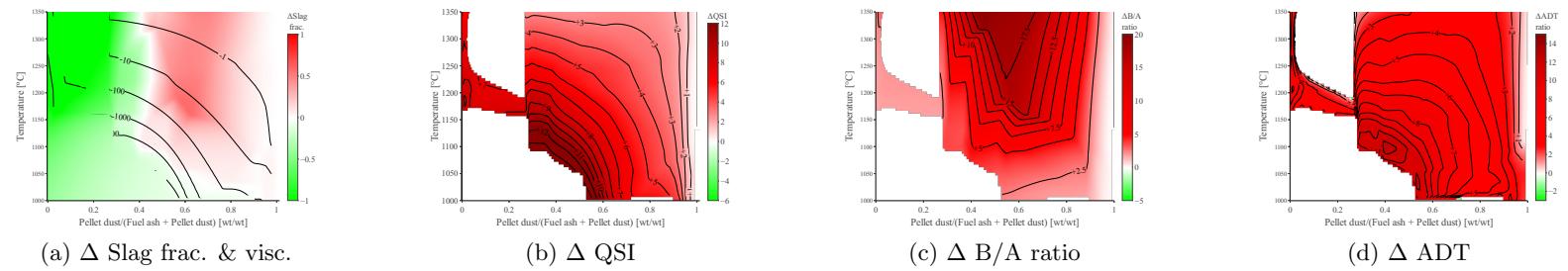


Figure S34: Bark difference (coal reference) plots

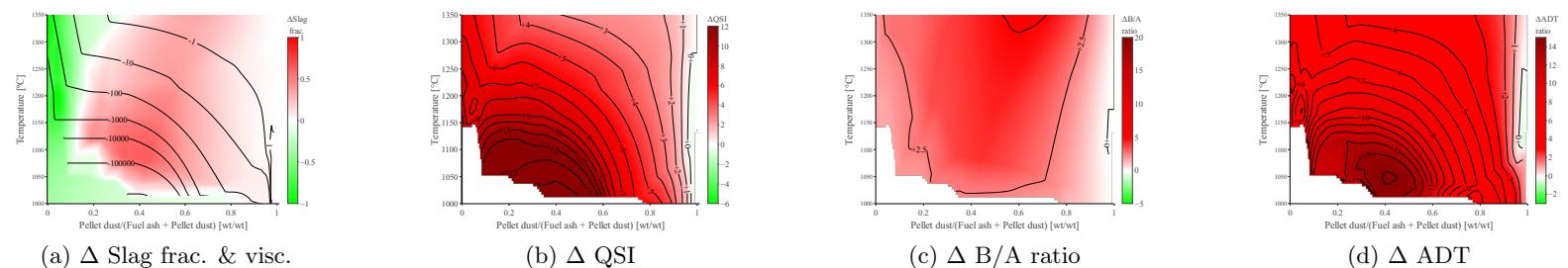


Figure S35: Forest residue difference (coal reference) plots

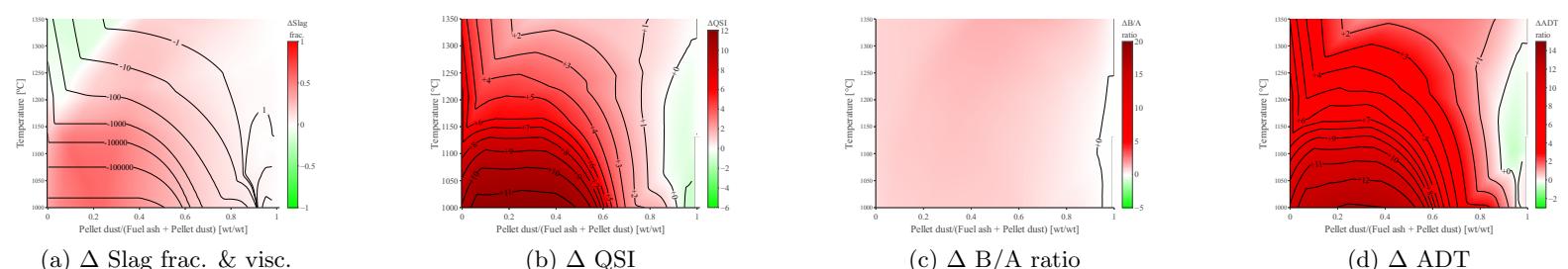


Figure S36: Reed-Canary-grass difference (coal reference) plots

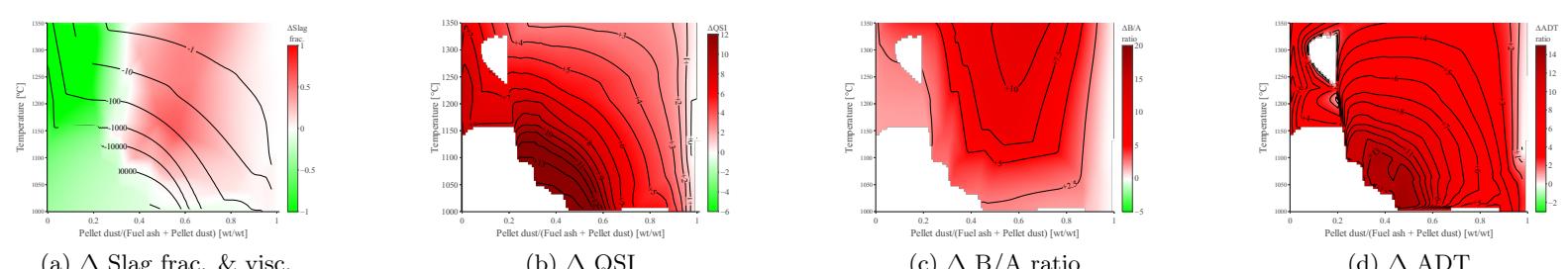


Figure S37: Willow difference (coal reference) plots

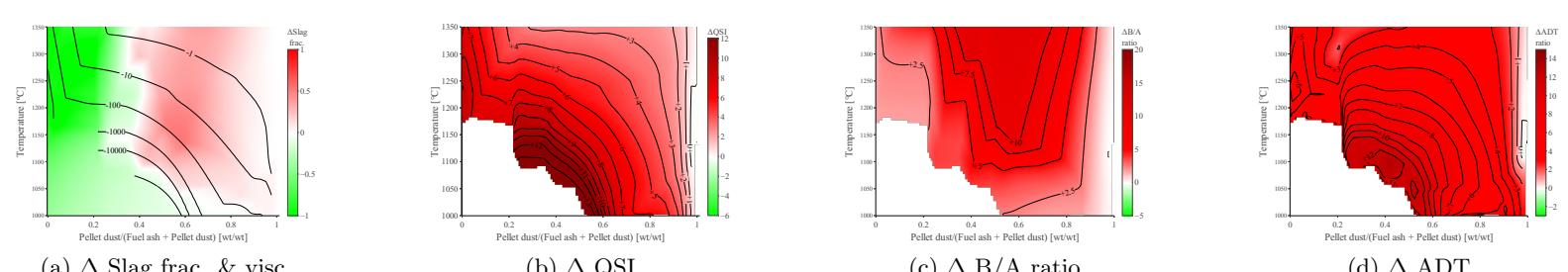


Figure S38: Stemwood difference (coal reference) plots

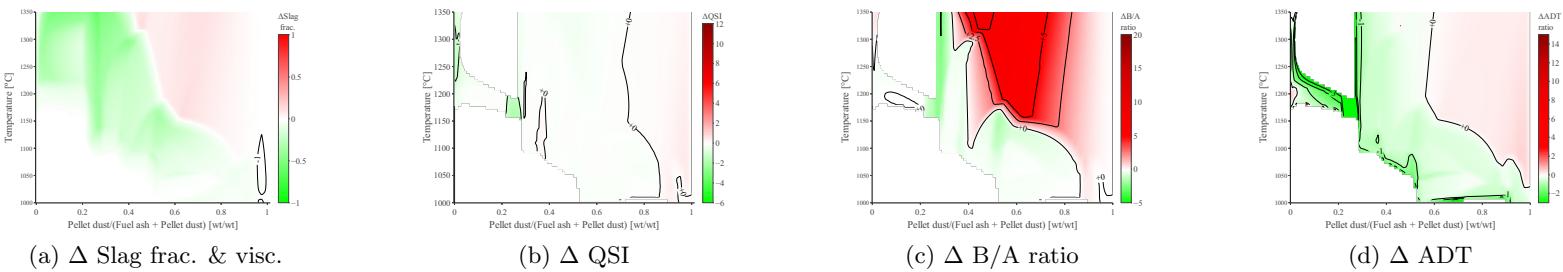


Figure S39: Bark difference (Biochar reference) plots

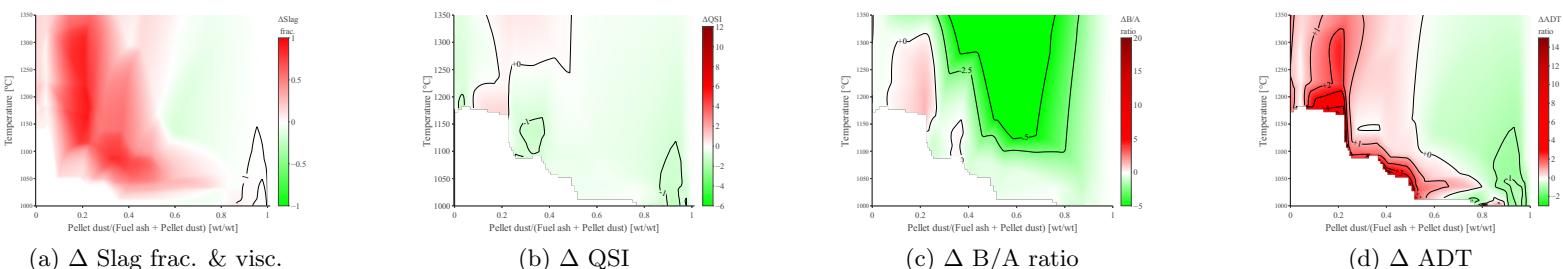


Figure S40: Forest residue difference (Biochar reference) plots

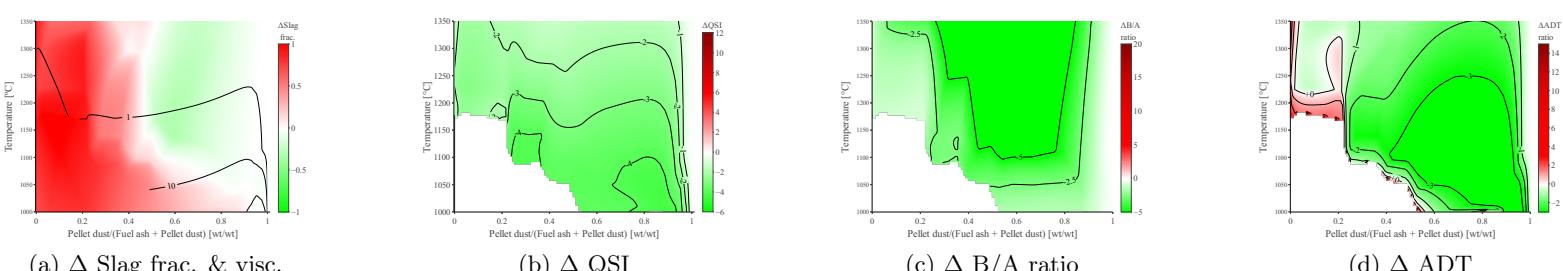


Figure S41: Reed-Canary-grass difference (Biochar reference) plots

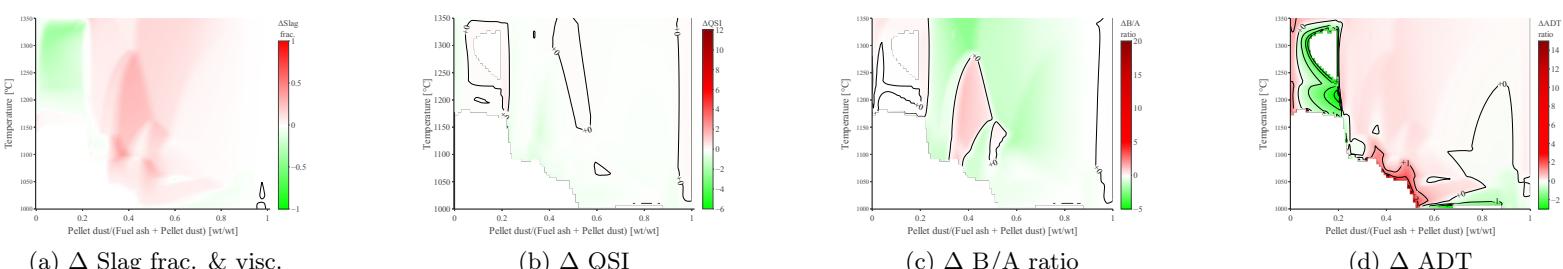


Figure S42: Willow difference (Biochar stemwood reference) plots

Section E_ Volatile behavior of ash

Description of the plot:

The total amount of vaporized ash (mg/MJ) for all the investigated fuels.

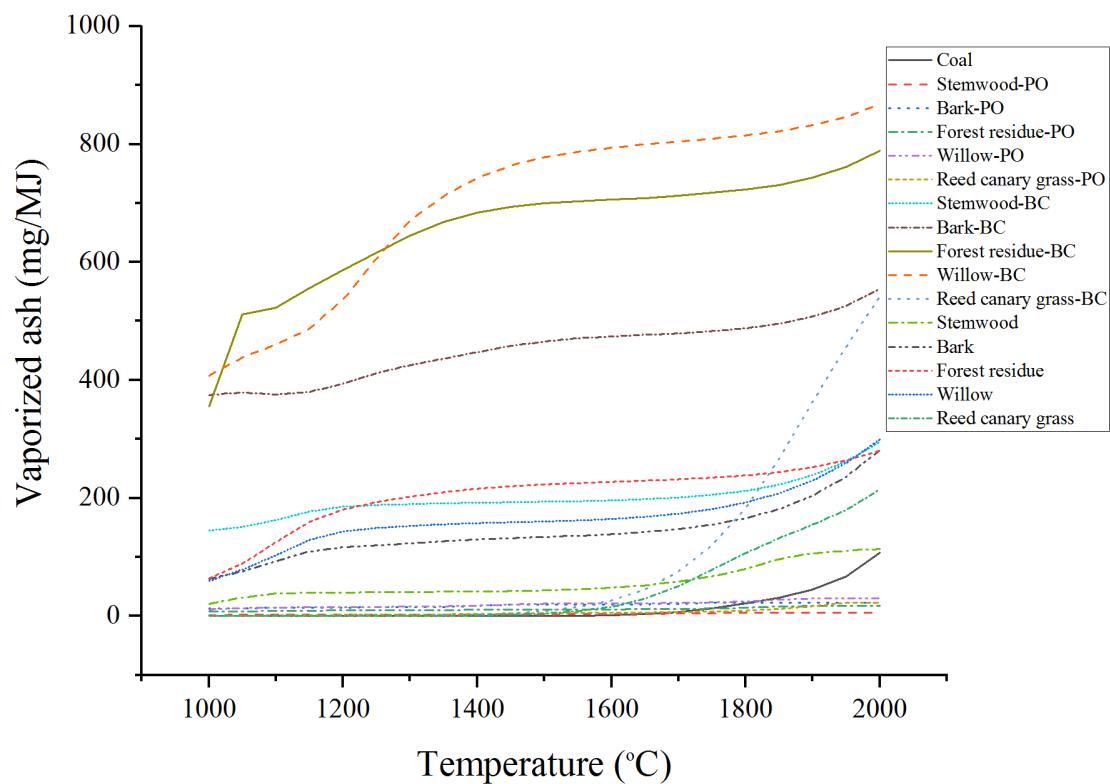


Figure S43: The total amount of vaporized ash (mg/MJ) for all the investigated fuels.