

Supplementary Material

S1. Bio-oil Composition

	C	H	O
Ultimate analysis, mol fraction ^a	0.286	0.491	0.223
Model mixture, mol fraction	0.268	0.519	0.213
Percentage of error, %	6.2	5.8	4.8
Water, wt.% ^a		24.3	
Model water, wt.%		24.0	
Family ^b	Family wt.%	Model compounds	Mass fraction
1	F1=10%	Formaldehyde, CH ₂ O	0.08
		Acetaldehyde, C ₂ H ₄ O	0.01
		1-hydroxy-2-butanone, C ₄ H ₈ O ₂	0.01
2	F2=30%	Acetic acid, C ₂ H ₄ O ₂	0.07
		Water, H ₂ O	0.23
3	F3=15%	Furfural, C ₅ H ₄ O ₂	0.13
		Phenol, C ₆ H ₆ O	0.01
		Water, H ₂ O	0.01
4	F4=15%	Creosol, C ₈ H ₁₀ O ₂	0.14
		Guaiacol, C ₇ H ₈ O ₂	0.01
5	F5+F6=30%	Catechol, C ₆ H ₆ O ₂	0.24
6		Palmitic acid, C ₁₆ H ₃₂ O ₂	0.01
		Levogluconan, C ₆ H ₁₀ O ₅	0.05
^a Composition of real PEFB bio-oil is from Pimenidou and Dupont [24]			
^b Macro-families are based on Garcia-Perez [27]			

S2. Equations for bare module cost of equipment

Process vessels	$C_{BM} = C_P^o F_{BM} = C_P^o (B_1 + B_2 F_M F_P)$
Heat exchangers	$C_{BM} = C_P^o F_{BM} = C_P^o (B_1 + B_2 F_M F_P)$
Pumps	$C_{BM} = C_P^o F_{BM} = C_P^o (B_1 + B_2 F_M F_P)$
Fans with electric drives	$C_{BM} = C_P^o F_{BM} F_P$
Fired heaters and furnaces	$C_{BM} = C_P^o F_{BM} F_P F_T$
Power recovery equipment	$C_{BM} = C_P^o F_{BM}$
Compressors and blowers without drives	$C_{BM} = C_P^o F_{BM}$
Drives for compressors and blowers	$C_{BM} = C_P^o F_{BM}$

C_{BM} is the bare module cost for each equipment type. F_M is the material factor, given for each equipment type in [35]. Those parts of the process that were exposed to bio-oil were assumed to be stainless steel, due to the corrosive nature of bio-oil [51]. Remaining parts of the process were assumed to be carbon steel. F_{BM} is the bare module factor, also given in [35]. F_T is a superheat correction factor for steam boilers, given by:

$$F_T = 1 + 0.00184\Delta T - 0.00000335(\Delta T)^2$$

Where ΔT is the amount of superheat of °C. $F_T = 1$ for other heaters and furnaces.

For process vessels, the pressure factor F_p was based on the ASME code for pressure vessel design:

$$F_{p,vessel} = \frac{\frac{(P_{vessel} + 1)D}{2[850 - 0.6(P_{vessel} + 1)]} + 0.00315}{0.0063} \text{ for } t_{vessel} > 0.0063m$$

where P_{vessel} is the operating pressure in barg, D is vessel diameter, and t_{vessel} is the wall thickness.

For remaining process equipment, F_p was calculated by:

$$\log_{10} F_p = C_1 + C_2 \log_{10}(P_{vessel}) + C_3 [\log_{10}(P_{vessel})]^2$$

where the constants C were taken from [35].

S3. Reactor Design

The reactor vessels consist of a steel shell with a refractory lining (**Figure S.3.1**).

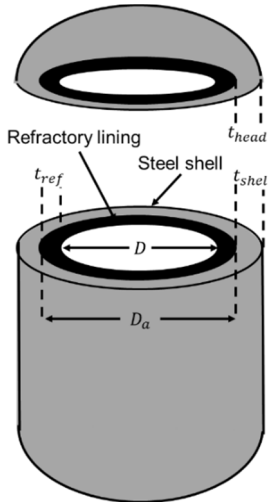


Figure S.3.1 Illustration of reactor vessel design

First, the volume of the reactors was estimated on the basis of the catalyst weight hourly space velocity (WHSV) and the sorbent quantity:

$$m_{cat} = \frac{WHSV}{\dot{m}_{bio-oil}}$$

$$m_{cat} = m_{sorb} X_{cat/sorb}$$

$$V = \left(\frac{m_{cat}}{\rho_{cat}} + \frac{m_{sorb}}{\rho_{sorb}} \right) (1 - \varepsilon_{bed})$$

Where m_{cat} and m_{sorb} are the mass of catalyst and sorbent respectively, and $\dot{m}_{bio-oil}$ is the mass flowrate of bio-oil in the reforming step, in kg h⁻¹. $X_{cat/sorb}$ is the mass ratio of catalyst to sorbent, taken from the process simulation. ρ_{cat} and ρ_{sorb} are the densities of catalyst and

sorbent respectively, and ε_{bed} is the bed void fraction. From this volume and the L/D ratio, the internal diameter T and the length U were calculated.

The thickness of refractory lining was calculated from an energy balance over the material [38]:

$$Q = \frac{2\pi\lambda L}{\ln(D_a/D)} (T_{max,cycle} - T_{steel})$$

where Q is the heat loss from each reactor, and λ is the thermal conductivity of refractory material. L is the reactor length, D_a is the internal diameter of refractory, and D is the internal diameter of the steel. $T_{max,cycle}$ is the maximum operating temperature in the SE-CLSR cycle, and T_{steel} is the maximum temperature the steel is exposed to. It was assumed that total heat losses were equal to 0.25% of the total heat production, that T_{steel} was 300°C, and λ was 0.2 W (m K)⁻¹ [38].

The wall thickness of the steel vessel was calculated from equations in Peters et al. [37], based on the ASME Boiler and Pressure Vessel Code.

For cylindrical shell:
$$t_{shell} = \frac{Pr_i}{SE_j - 0.6P} + C_c$$

For a hemi-spherical head:
$$t_{head} = \frac{PL_a}{2SE_j - 0.2P} + C_c$$

The terms in the equations were defined as follows:

t_{vessel}	Minimum wall thickness	m
P	Maximum allowable internal pressure	kPa
r_i	Inside radius of the shell, before corrosion allowance is added	m
S	Maximum allowable working stress	kPa
E_j	Efficiency of joints, expressed as a fraction	-
C_c	Corrosion allowance	m
L_a	Inside radius of hemispherical head	m

The mass of the shells were calculated using the volume of a hollow cylinder:

$$m_{cylinder} = \rho_m \pi L (\pi r_o^2 - \pi r_i^2)$$

The mass of each hemi-spherical head was given by [37]:

$$m_{head} = \rho_m [2\pi L_a^2 t_{head}]$$

The total mass of steel and of refractory was given by:

$$m_{steel} = f(m_{cylinder,steel} + 2m_{head,steel})$$

$$m_{ref} = m_{cylinder,ref} + 2m_{head,ref}$$

where the factor f was used to account for the extra mass of vessel hardware. For horizontal vessels, f was assumed to be 1.015, and for vertical vessels, f was assumed to be 1.2 [37]. SE-CLSR reactors were assumed to be vertical vessels.

Having found the mass of steel and refractory, the total cost of the reactor was:

$$C_P^0 = C_{steel} + C_{ref}$$

where C_{steel} and C_{ref} are the cost of steel and refractory respectively.

The cost of the steel vessel was calculated from Peters et al. [37], while the cost of refractory was calculated on a simple mass basis:

$$C_{steel} = 73m_{steel}^{-0.34}$$

$$C_{ref} = P_{ref}(m_{cylinder,ref} + m_{head,ref})$$

where P_{ref} is the price of refractory material \$ kg⁻¹.

According to Peters et al. [37], Eq B.12 is valid over a range of 400 to 50,000 kg. When the calculated mass of steel exceeded 50 tonnes, the total required volume was divided into smaller reactors until this threshold was met.

The total bare module cost was then found using the equation from Turton et al. [35]:

$$C_{BM} = C_P^0 F_M F_P$$

The pressure factor F_P was equal to 1, as the calculation had accounted for pressure. The material factor F_M for a stainless steel vessel was 3.2 [37].