Entrained flow reactor (EFR)

Gavin Wiggins

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1 Introduction

This report provides an overview of the Entrained Flow Reactor (EFR) at NREL and associated computational modeling tasks. The reactor operates at fast pyrolysis conditions to thermochemically convert biomass into gaseous products. The EFR is part of the Thermochemical Process Development Unit (TCPDU) at NREL which was originally designed for biomass gasification where the EFR was used as a thermal cracker. An overview of the TCPDU system is shown in Figure 1.

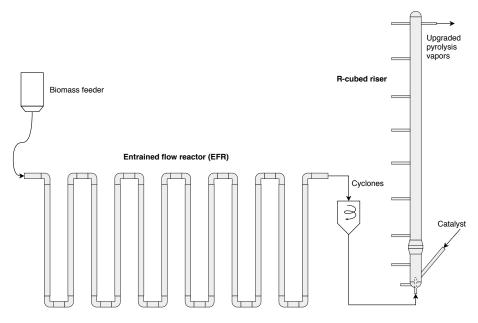


Figure 1: Overview of the main components of the NREL TCPDU system. Fast pyrolysis of biomass occurs in the entrained flow reactor. Catalytic vapor phase upgrading occurs in the R-cubed riser reactor.

2 Experimental setup

This section provides geometric dimensions and typical operating conditions for the entrained flow reactor. Characteristics for the Blend3 and forest residue feedstocks are also discussed.

2.1 Entrained flow reactor

Fast pyrolysis in the TCPDU system occurs in the entrained flow reactor (EFR) which is comprised of a series of horizontal and vertical pipes connected with 90 degree elbows (see Figure 2). The EFR is essentially a pneumatic conveyor where biomass particles flow through a long pipe with several bends. Dimensions and material information about the EFR are provided in Figure 3 below. Operating conditions such as temperatures, pressures, and flow rates for the EFR are shown in Figure 4. Nitrogen gas at 500°C is generally used as the conveying medium for the solids.

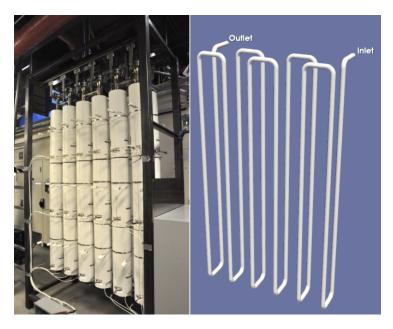


Figure 2: Left - picture of the EFR assembly with heat jackets, insulation, and thermocouples. Right - CAD representation of the EFR pipe assembly used for MFiX simulations.

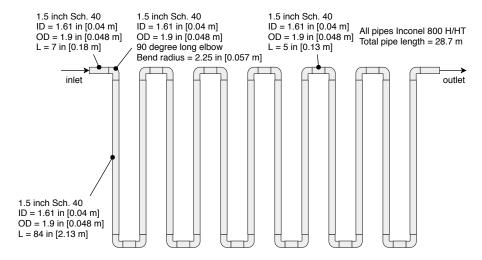


Figure 3: Geometry of the entrained flow reactor at NREL.

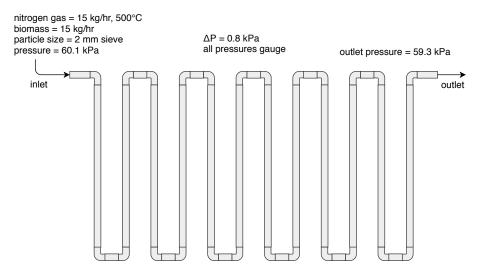


Figure 4: Typical operating conditions for the entrained flow reactor.

2.2 Blend3 feedstock

General information about the Blend3 feedstock used in the entrained flow reactor is provided in Table 1. There is currently no information regarding identification of the feedstock or who performed the feedstock measurements and data preparation. Proximate and ultimate analysis data for the feedstock are presented in Tables 2 and 3. Only one set of analysis data is available therefore the uncertainty in the values is unknown.

Table 1: General information for the Blend3 feedstock.

Item	Description
Name	Blend3
ID	?
Contact	?

Table 2: Blend3 proximate analysis mass percent, as-received basis. Source [3].

Proximate	%ar	%ar	%ar
FC	16.92	?	?
VM	76.40	?	?
ash	0.64	?	?
moisture	6.04	?	?

Table 3: Blend3 ultimate analysis mass percent, as-received basis. Source [3].

Element	% ar	% ar	% ar
С	49.52	?	?
H	5.28	?	?
O	38.35	?	?
N	0.15	?	?
\mathbf{S}	0.02	?	?
ash	0.64	?	?
moisture	6.04	?	?

The chemical analysis of the Blend3 feedstock is presented in Table 4. Again, only one set of data is available so the uncertainty in the measurements is unknown. The chemical analysis measurements are used to determine the biomass composition which is needed for the kinetics model.

Table 4: Blend3 chemical analysis mass percent, dry basis. Source [6].

Chemical component	% dry	% dry	% dry
glucan	38.95	?	?
acetyl	1.59	?	?
arabinan	1.40	?	?
galactan	3.16	?	?
mannan	10.52	?	?
xylan	7.89	?	?
lignin	29.48	?	?
free fructose	0.07	?	?
free glucose	0.04	?	?
sucrose	0.04	?	?
water extractives	2.75	?	?
ethanol extractives	3.49	?	?
non-structural inorganics	0.22	?	?
structural inorganics	0.41	?	?

Table 5: Blend3 ash analysis as weight percent of ash. Source [3].

Metal oxide	wt. %	wt. %	wt. %
-SiO ₂	28.1	?	?
Al_2O_3	7.06	?	?
${ m TiO_2}$	0.34	?	?
CaO	21.8	?	?
Na_2O	0.71	?	?
K_2O	13.8	?	?
P_2O_5	5.47	?	?
SO_3	1.23	?	?
Cl	0.09	?	?
CO_2	5.14	?	?

Table 6: Blend3 particle properties from pelletized crushed feedstock. The crushed feedstock is used in the entrained flow reactor.

Property	Value	Description	Source
ρ	$1{,}050~\rm kg/m^3$	particle density, daf basis	[5]
η	0.27	particle porosity	
k	$0.23~\mathrm{W/mK}$	thermal conductivity	

Table 7: Entrained flow reactor yields for Blend3 feedstock.

Yield	wt. %
total liquid	64.9
char	13.9 ± 0.1
gas	17.2 ± 0.2
mass balance	96.9 ± 1.5
carbon balance	93.0 ± 1.0

2.3 Forest residue feedstock

The forest residue feedstock is comprised of branches/twigs, cambium, needles, bark, and whitewood. This feedstock is used in the NREL fluidized bed reactor (FBR) for the purposes of the FCIC project. The FBR is operated at fast pyrolysis conditions for the thermochemical conversion of biomass. The reactor is sometimes referred to as the 2FBR.

Table 8: General information for the forest residue feedstock.

Item	Description
Name	forest residue
ID	?
Contact	?

Table 9: Bark ultimate analysis mass percent, dry ash-free basis. Source [1].

Element	% daf	% daf	% daf
С	48.27	?	?
H	5.72	?	?
N	0.52	?	?

Table 10: Branches/twigs ultimate analysis mass percent, dry ash-free basis. Source [1].

Element	% daf	% daf	% daf
С	49.69	?	?
Н	6.36	?	?
N	0.25	?	?

Table 11: Cambium ultimate analysis mass percent, dry ash-free basis. Source [1].

Element	% daf	% daf	% daf
С	48.52	?	?
H	6.39	?	?
N	0.11	?	?

Table 12: Needles ultimate analysis mass percent, dry ash-free basis. Source [1].

Element	% daf	% daf	% daf
С	48.59	?	?
H	5.92	?	?
N	1.22	?	?

Table 13: Whitewood ultimate analysis mass percent, dry ash-free basis. Source [1].

Element	% daf	% daf	% daf
С	48.27	?	?
\mathbf{H}	6.15	?	?
N	0.10	?	?

Table 14: Whitewood biomass composition mass percent, dry basis. Source [2].

Component	% dry
Cellulose	38.04
Hemicellulose	24.2

3 Model development

 $\qquad \qquad \text{Here.}$

3.1 Biomass pyrolysis kinetics

The Debiagi et al. [4] kinetic scheme for biomass pyrolysis is discussed in this section.

Table 15: Solid species in the Debiagi kinetic scheme.

Item	Abbreviation	Name	Formula
1	CELL	cellulose	$C_6H_{10}O_5$
2	CELLA	activated cellulose	$C_6H_{10}O_5$
3	CHAR	char	\mathbf{C}
4	GCO	metaplastic carbon monoxide	CO
5	GCO2	metaplastic carbon dioxide	CO_2
6	GCH4	metaplastic methane	CH_4
7	GC2H4	metaplastic ethylene	C_2H_4
8	GCH3OH	metaplastic methyl alcohol	$\mathrm{CH_{4}O}$
9	GCOH2	metaplastic formaldehyde	$\mathrm{CH_{2}O}$
10	GH2	metaplastic hydrogen	H_2
11	GMSW	hemicellulose softwood	$C_5H_8O_4$
12	HCE1	hemicellulose	$C_5H_8O_4$
13	HCE2	hemicellulose	$C_5H_8O_4$
9	HMWL	heavy molecular weight lignin	$\mathrm{C}_{24}\mathrm{H}_{28}\mathrm{O}_4$
14	LIG	lignin	$\mathrm{C}_{11}\mathrm{H}_{12}\mathrm{O}_4$
15	LIGC	lignin carbon	$\mathrm{C}_{15}\mathrm{H}_{14}\mathrm{O}_4$
16	LIGCC	lignin carbon	$\mathrm{C}_{15}\mathrm{H}_{14}\mathrm{O}_4$
17	LIGH	lignin hydrogen	$\mathrm{C}_{22}\mathrm{H}_{28}\mathrm{O}_{9}$
18	LIGO	lignin oxygen	$C_{20}H_{22}O_{10}$
19	LIGOH	lignin hydroxide	$\mathrm{C}_{19}\mathrm{H}_{22}\mathrm{O}_{8}$
20	XYHW	hemicellulose hardwood	$C_5H_8O_4$

Table 16: Gas species in the Debiagi kinetic scheme.

Item	Abbreviation	Name	Formula
1	ACAC	acetic acid	$C_2H_4O_2$
2	ALD3	propanal	C_3H_6O
3	ANISOLE	anisole	C_7H_8O
4	C2H4	ethylene	C_2H_4
5	C2H6	ethane	C_2H_6
6	C2H5OH	ethanol	C_2H_6O
7	C2H3CHO	2-propenal	C_3H_4O
8	C3H6O2	propanal, 3-hydroxy-	$C_3H_6O_2$
9	CH2O	formaldehyde	$\mathrm{CH_{2}O}$
10	СНЗОН	methyl alcohol	$\mathrm{CH_{4}O}$
11	СНЗСНО	acetaldehyde	C_2H_4O
12	CH4	methane	CH_4
13	CO	carbon monoxide	CO
14	CO2	carbon dioxide	CO_2
15	COUMARYL	coumaryl alcohol	$C_9H_{10}O_2$
16	FE2MACR	sinapaldehyde	$C_{11}H_{12}O_4$
17	FURF	furfural	$C_5H_4O_2$
18	GLYOX	glyoxal	$C_2H_2O_2$
19	H2	hydrogen	H_2
20	H2O	water	H_2O
21	HAA	hydroxy-acetaldehyde	$C_2H_4O_2$
22	HCOOH	formic acid	$\mathrm{CH_2O_2}$
23	HMFU	5-hydroxymethyl-furfural	$C_6H_6O_3$
24	LVG	levoglucosan	$C_6H_{10}O_5$
25	PHENOL	phenol	C_6H_6O
26	XYLAN	xylosan	$C_5H_8O_4$

3.2 Biomass characterization

Here.

Table 17: Blend3 biomass composition mass percent, dry basis. Values are calculated from Table 4.

Biomass composition	% dry
cellulose	38.95
hemicellulose	24.56
lignin	29.48
tann	2.90
tgl	3.49
ash	0.63

4 Results and discussion

Here.

5 Conclusions

Here.

6 Source code

The Python code used to develop the models and generate results discussed in this paper is available on GitHub at https://github.com/ccpcode/nrel-efr.

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