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Comparative kinetic analysis of furfural production from xylan and xylose

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Overview

- Introduction
- Aims and objectives
- Methodology
- Modelling
- Results and discussions
- Conclusion

Introduction (Background)

- Furfural is a valuable platform chemical with extensive applications as a bio alternative for petrochemicals.
- Applications of furfural;

Fuel

Plastics

Solvents

Introduction (Background)

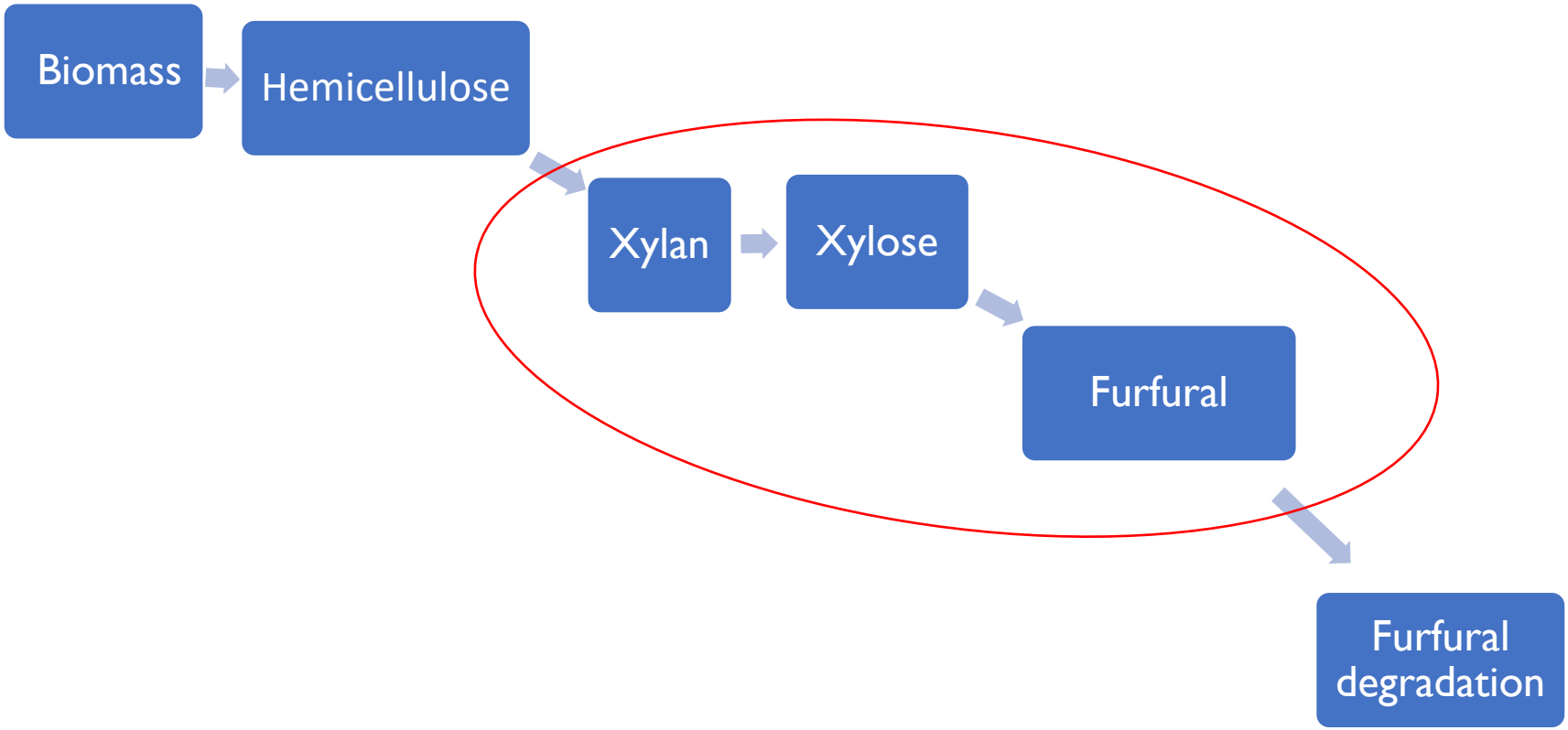
- Furfural is derived from the hemicellulose of some hard wood lignocellulose biomass
- Two methods of furfural production
  1. Direct method- Acid catalyzed conversion of untreated lignocellulose
  2. Indirect method- Acid catalyzed conversion of pre-treated feed materials
- Pre-treated feed materials
  1. Hemicellulose hydrolysate- fractionated hemicellulose component
  2. Xylan - polymeric component of the hemicellulose converted to furfural
  3. Xylose -monomeric pentose compound

Introduction (Xylan Versus Xylose)

Xylan	Xylose
Polymeric compound	Monomeric compound
$(C_5H_{10}O_5)_n$ +side chains	$C_5H_{10}O_5$
Two step process	One step process
No relevant kinetic study	Significant kinetic study

- This study will provide critical information on the kinetics of furfural formation from pre-extracted xylan and further on the comparison of the kinetics of furfural production from xylan and xylose

Introduction(Furfural production overview)



Aims and objectives

AIM

- To analyze and compare the kinetics of furfural formation from xylan and xylose

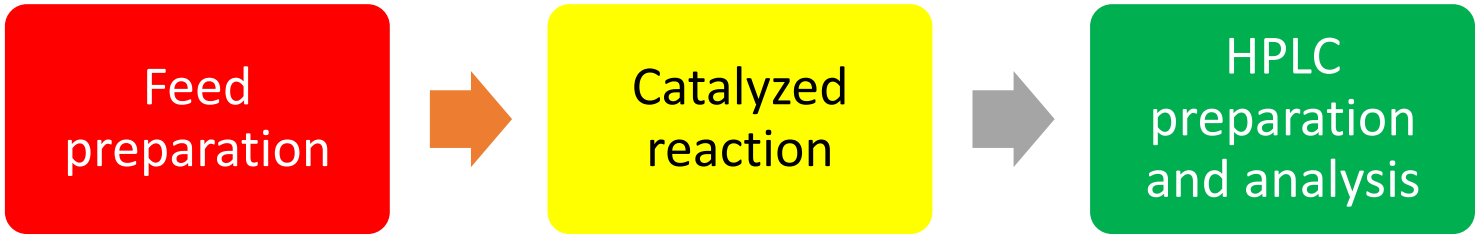
OBJECTIVES

- To examine separate experimental data for xylan and xylose conversion to furfural within a specified range of conditions
- To select appropriate kinetics models from literature that best describes the experimental data
- To compare selected models for the two conversion processes

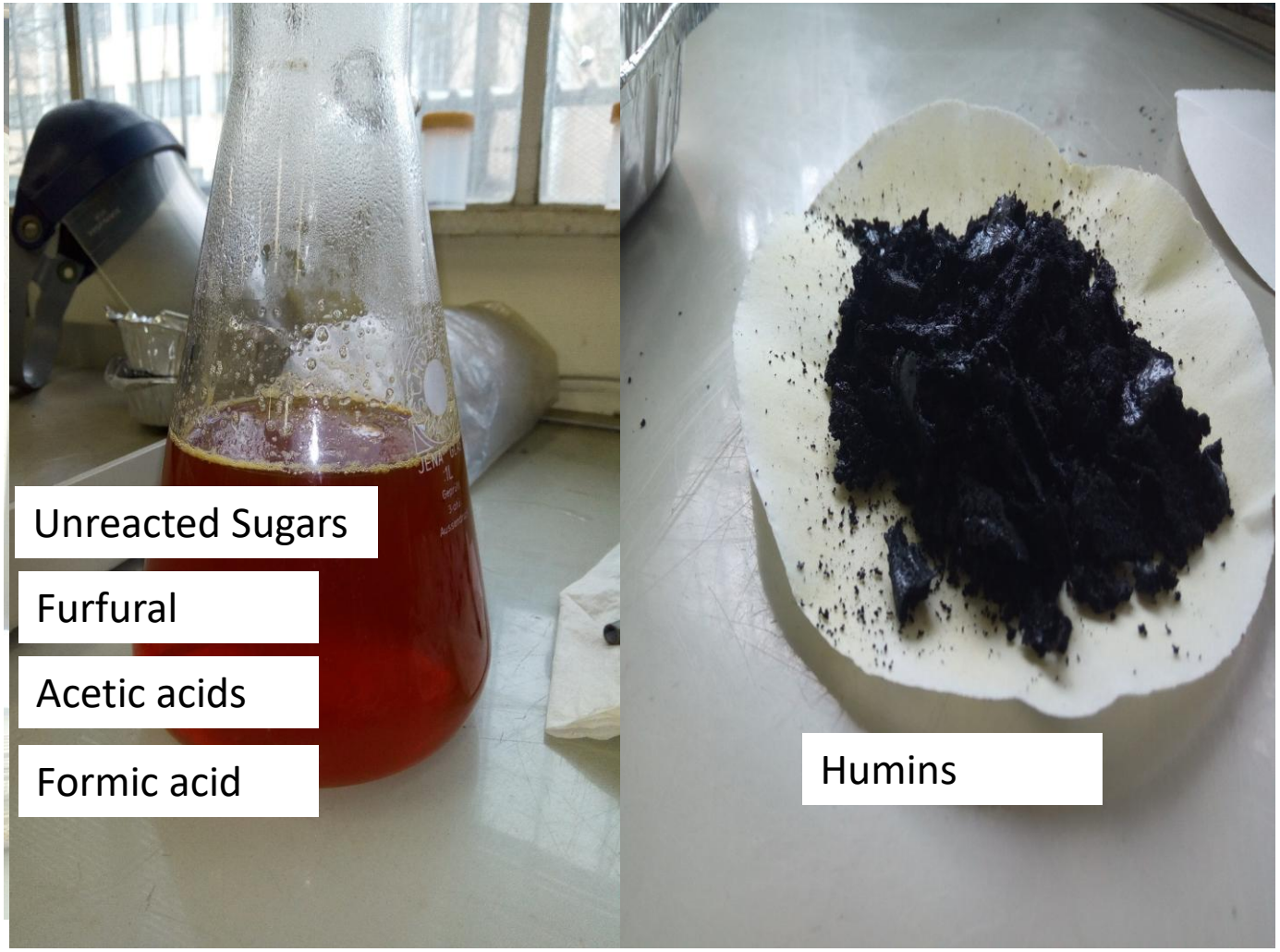
Methodology (Process selection)

Summary of experimental conditions

Conditions	Range		
	Low	Medium	High
Temperature (°C)	140	155	170
Acid concentration (wt %)	0.5	1	2
Solids loading (wt %)	4	8	14
Feed stock	Xylan and Xylose		

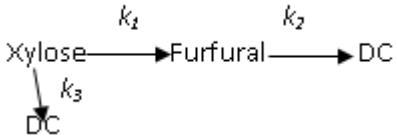


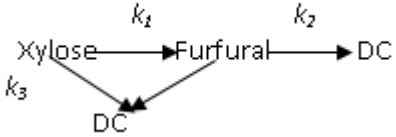
Methodology (Experimental set-up)



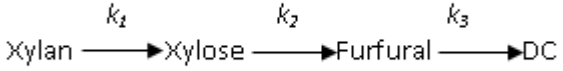
Methodology (Kinetics models)

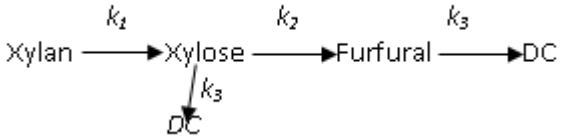
Xylose

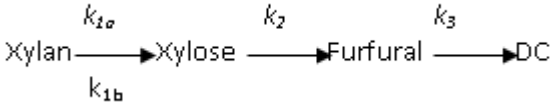


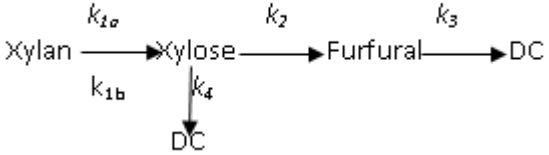


Xylan









Modelling

Spyder (Python 3.6)

File Edit Search Source Run Debug Consoles Projects Tools View Help

C:\Users\21424233

Editor - C:\Users\21424233\Python model\IRENE DATA\ALDATA regular - acid.py

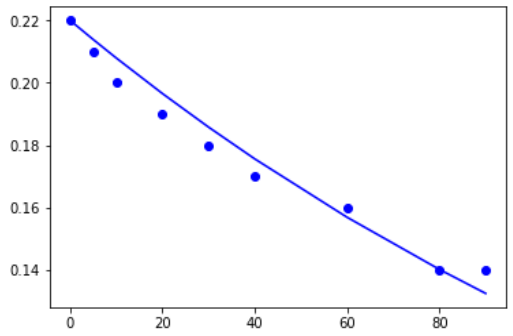
ALDATA regular - acid.py

```
xylose_data=np.zeros((9,27))
furf=np.zeros((9,27))
time=np.zeros((9,27))

#%%

for i in [0,1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24,25,26]:
    time[:,i] = data[:,(i*1)*3]
    xylose_data[:,i]=data[:,(i*3)+1]
    furf[:,i]=data[:,(i*3)+2]

#%%
#xylose_data=normalize(xylose_data,axis=0,norm="max")
#furf=normalize(furf,axis=0,norm="max")
Temperature=[140,140,140,140,140,140,140,140,140,155,155,155,155,155,155,155,155,155,170,170,
Ts=[i+273 for i in Temperature ] # all temps in Kelvin
Ac=[5.7e-2,1.1e-1,2.1e-1,5.7e-2,1.1e-1,2.1e-1,5.7e-2,1.1e-1,2.1e-1,5.7e-2,1.1e-1,2.1e-1,5.7e-
n = 9
w=27
fx0 = xylose_data[0,:]
ff0=furf[0,:]
R=8.314 # J/K*mol
#%%
# Arrhenius equation
def Arr(T,A1,E1,H):
    k1=H*A1*np.exp(-E1/(R*T))
    return k1
#%%
def squared_error(xo):
    global Mx
    global Mf
    global Md
    Mx = np.zeros((n,w))
    Mf = np.zeros((n,w))


    A1 = xo[0]
    E1 = xo[1]
```

IPython console

Console 1/A

```
X3= 0.78892966722
F3= 0.885295575722
X4= 0.653293674712
F4= 0.762720071372
X5= 0.738108761309
F5= 0.297887473738
X6= 0.762669065317
F6= 0.297107976564
X7= 0.877578189123
F7= 0.297344931119
X8= 0.855264583508
F8= 0.696590044231
X9= 0.978023704515
F9= 0.787528649575
X10= 0.593223748712
F10= 0.528813272893
X11= 0.541442221523
F11= 0.660278528163
X12= 0.952167384535
F12= 0.206473230732
```



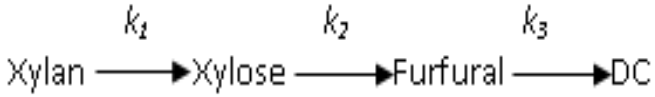
IPython console | Profiler | Variable explorer

Permissions: RW | End-of-lines: CRLF | Encoding: UTF-8 | Line: 301 | Column: 18 | Memory: 32 %

Results and discussion (Kinetics models and parameters)

- **Scheme 1 – Xylose conversion**

Scheme 2 –Xylan conversion



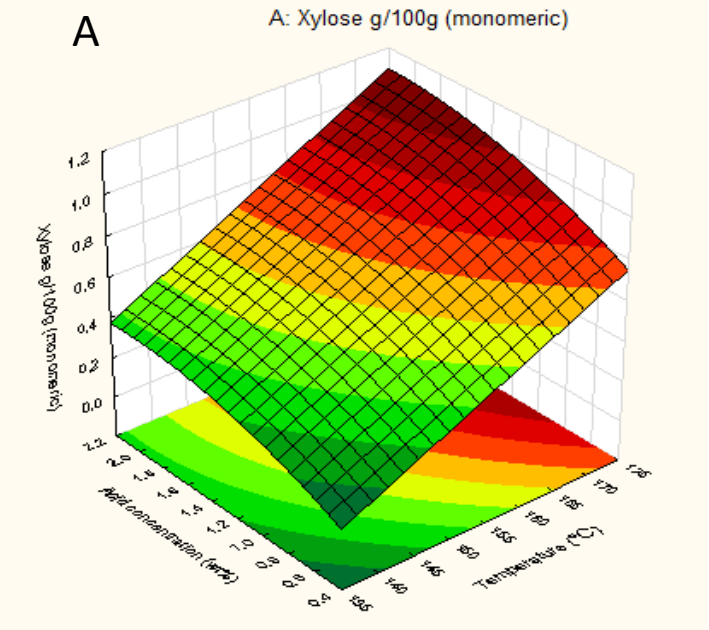
Feed	**k_0**		**k_1**		**k_2**	
	A	Ea (kJ/mol)	A	Ea (kJ/mol)	A	Ea (kJ/mol)
Xylan	7.75×10^8	55	2.96×10^{11}	98	1.20×10^{11}	120
Xylose	-	-	4.64×10^{10}	95	3.77×10^2	28

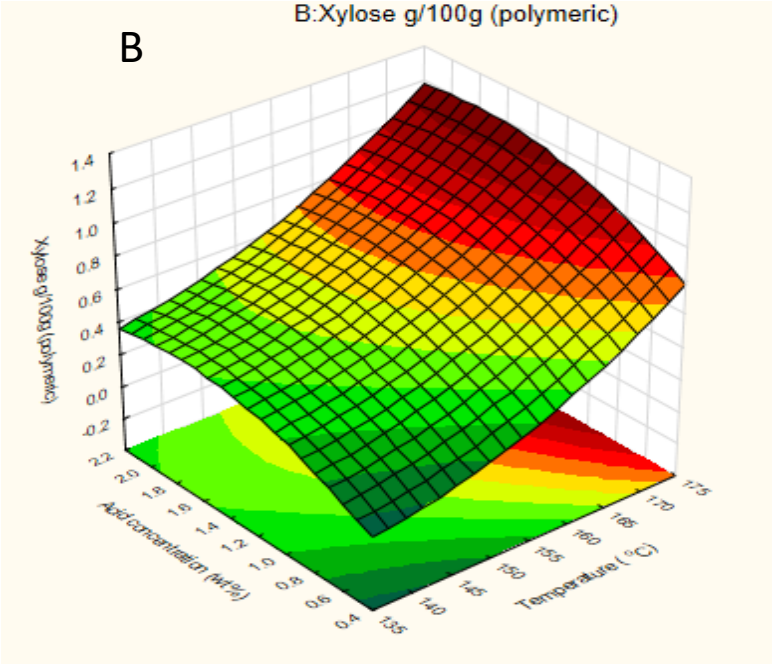
Results and discussion (Statistical analysis)

Variables	p-values			
	Xylose feed (g/100g)		Xylan feed (g/100g)	
	Xylose g/100g	Furfural g/100g	Xylose g/100g	Furfural g/100g
Temperature (°C) (T)	0.0000	0.0000	0.0000	0.0000
Solids Conc (wt%) (S)	0.5200	0.0400	0.4100	0.0660
Acid Conc (wt%) (A)	0.0000	0.0005	0.0000	0.0180
TXS	0.6000	0.0800	0.2400	0.6600
TXA	0.4770	0.1780	0.6500	0.0580
SXA	0.4800	0.6700	0.1900	0.1800
R^2	0.9600	0.8700	0.9300	0.7800

Results and discussion (Experimental conditions)

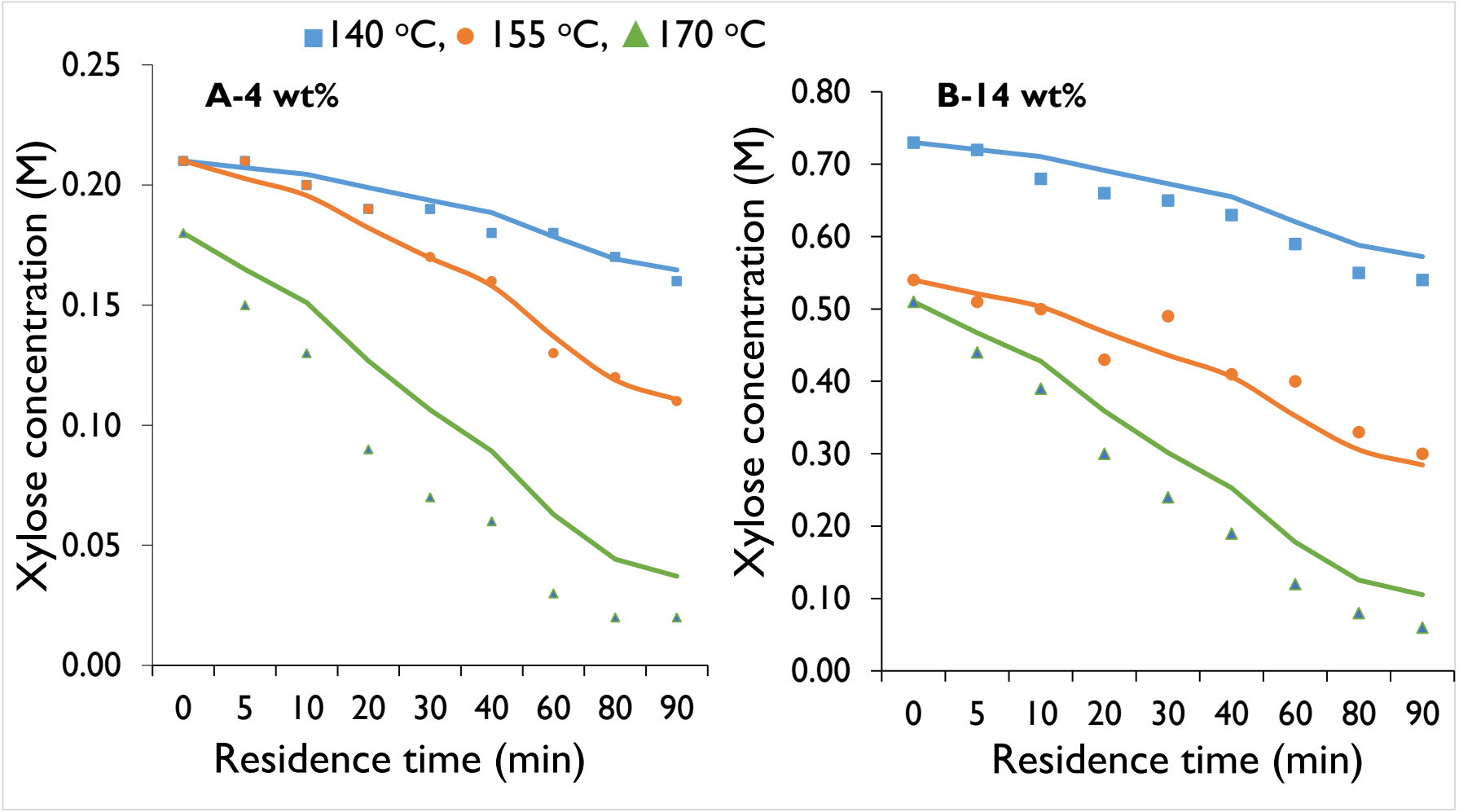
- Furfural production was found to be dependent on two main conditions
  - Temperature
  - Acid concentration





A-Xylose, B-Xylan

Results and discussion (Effect of experimental conditions)



Results and discussion (Side reactions)

- Products of reaction
  - Furfural
  - Humins
  - Formic acid
  - Acetic acid

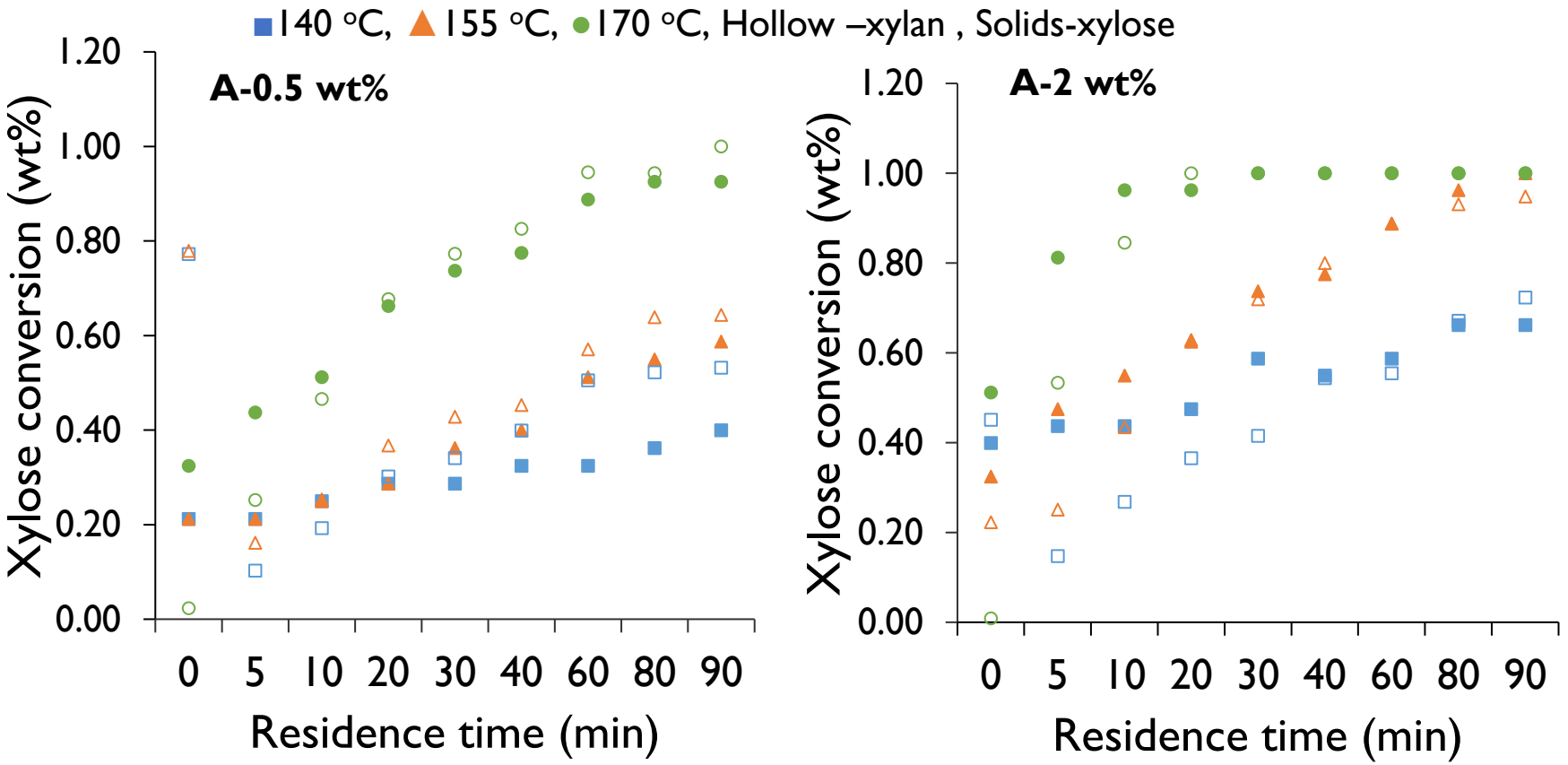
- Degradation reactions
  - Condensation reaction

Furfural + Pentose precursor (intermediate) ⟶ Furfural Pentose

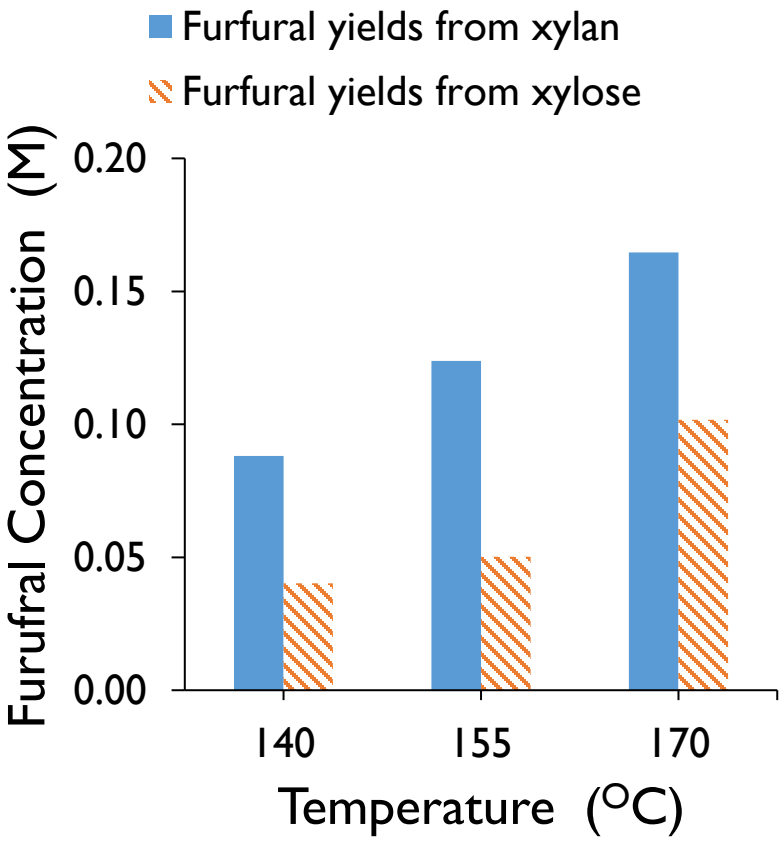
  - Resinification reaction

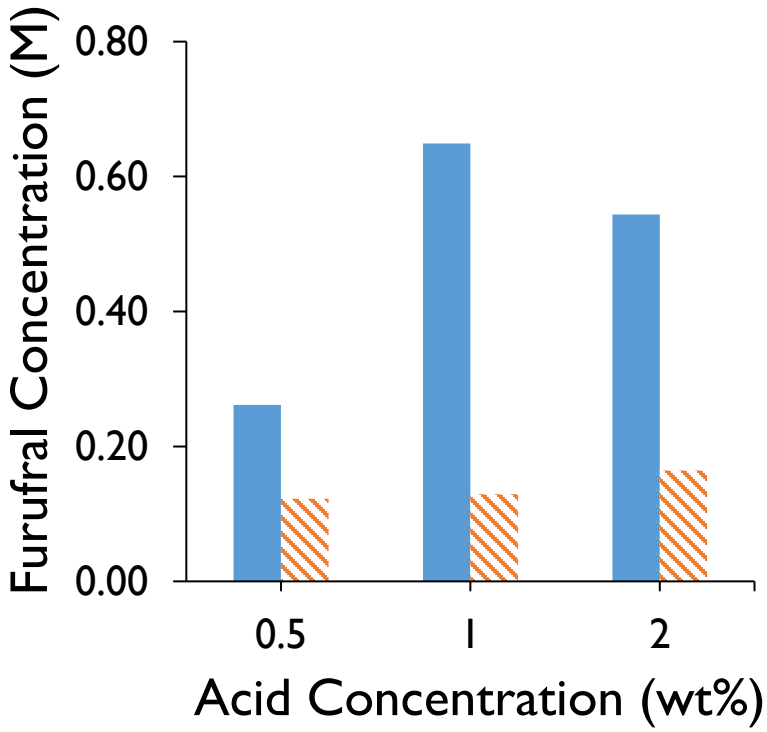
nFurfural ⟶ (Furfural)n

Results and discussion (Acid concentrations effect rate of conversions)



Results and discussion (Yields)





Conclusion

- Over all, the selected models described the reaction sufficiently.
- Both models determined there were no significant side reactions from xylan and xylose.
- Temperature and acid loading demonstrated significant effect on the reaction and the reaction mechanism.
- The xylan conversion process was generally faster due to the higher acid concentrations compared to the xylose conversion process.
- Finally, higher furfural yields were recorded for xylan compared to xylose at all conditions investigated in this study due to the extent of furfural degradation for the xylose feed reaction
- **Recommendations**
- Extend study to xylan from different plant sources

Acknowledgments

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- Colleagues and friends who have been there for me through this journey

Thank you!

Questions?