

Modélisation chimique détaillée de la combustion de la biomasse dans les appareils de chauffage domestique en vue de réduire leurs émissions polluantes

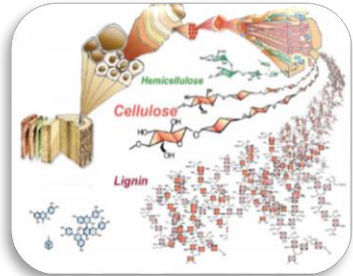
Amal DHAHAK

Encadré par : Frédérique BATTIN-LECLERC¹, Roda BOUNACEUR¹, Olivier HERBINET¹,
Céline LE DREFF²

Correspondant ADEME: Florence PROHARAM³

1: LRGP, 2: CSTB, 3: ADEME

Plan

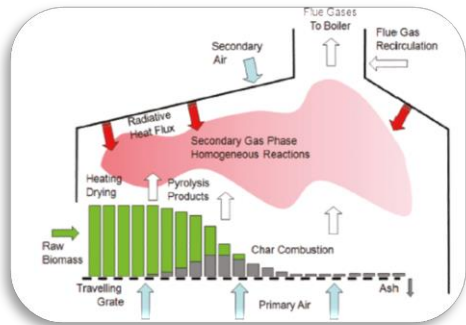
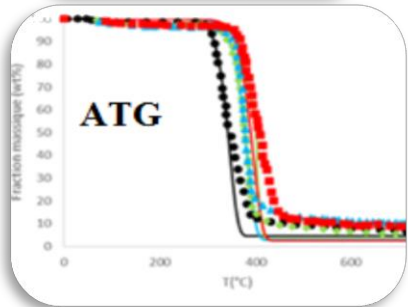


- 1- Introduction et contexte général

- 2- Démarche adoptée

- 3- Résultats

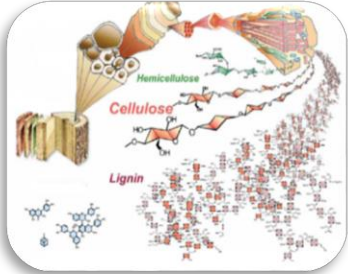
- 4- Conclusion et perspectives



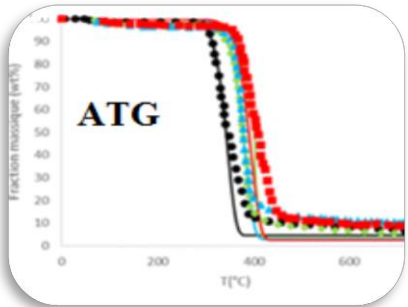
Plan



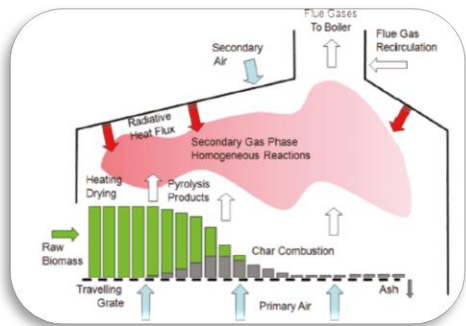
- 1- Introduction et contexte général



- 2- Démarche adoptée



- 3- Résultats

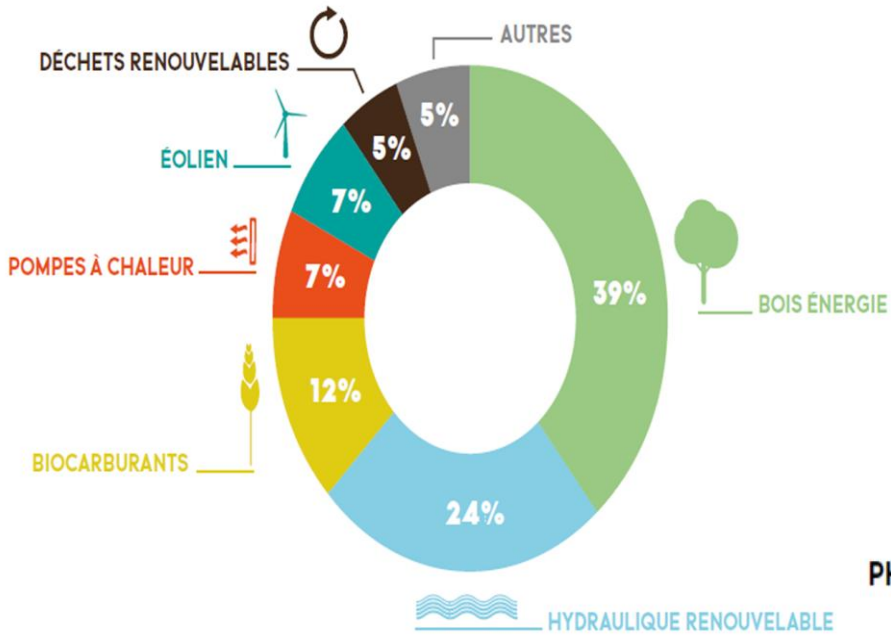


- 4- Conclusion et perspectives

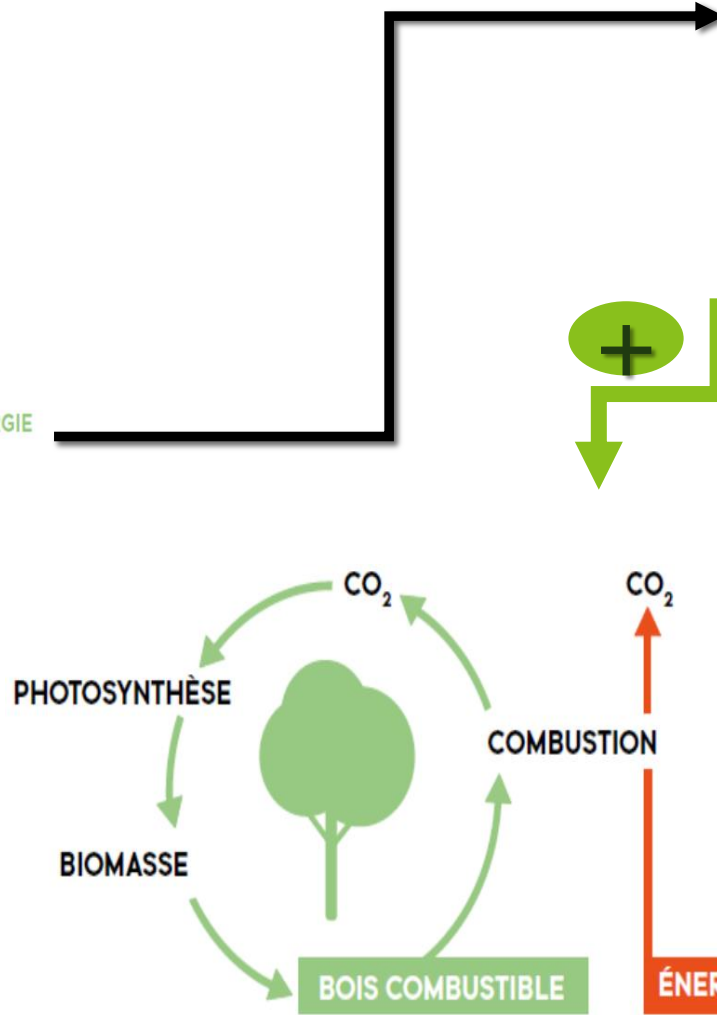


1. Introduction et contexte général

PRODUCTION PRIMAIRE D'ÉNERGIES RENOUVELABLES EN FRANCE EN 2014

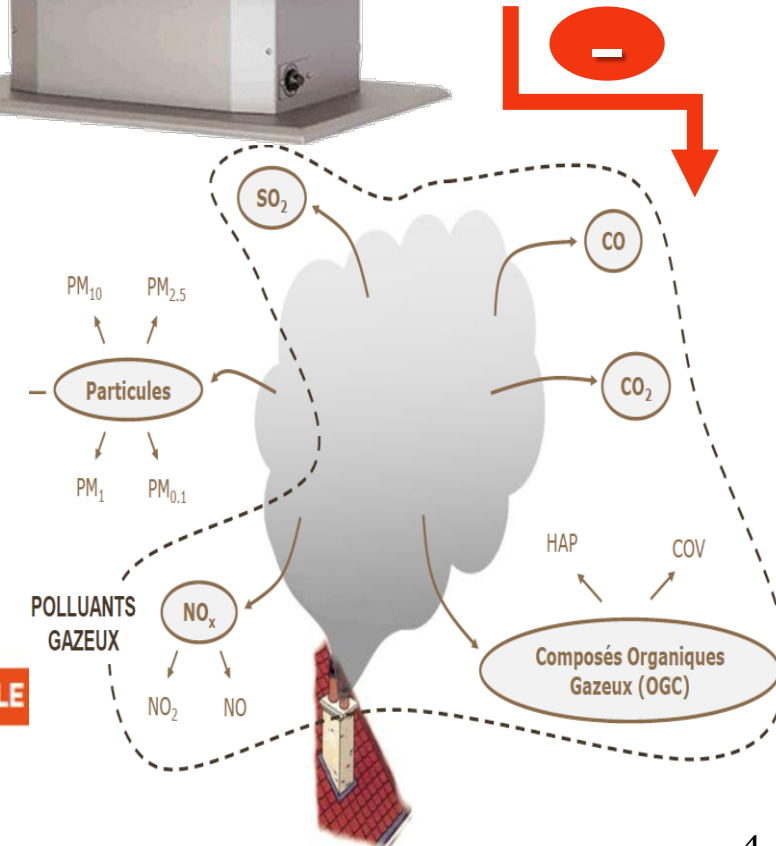


Source : CGDD-SOES



LE CYCLE CARBONE DU BOIS ÉNERGIE

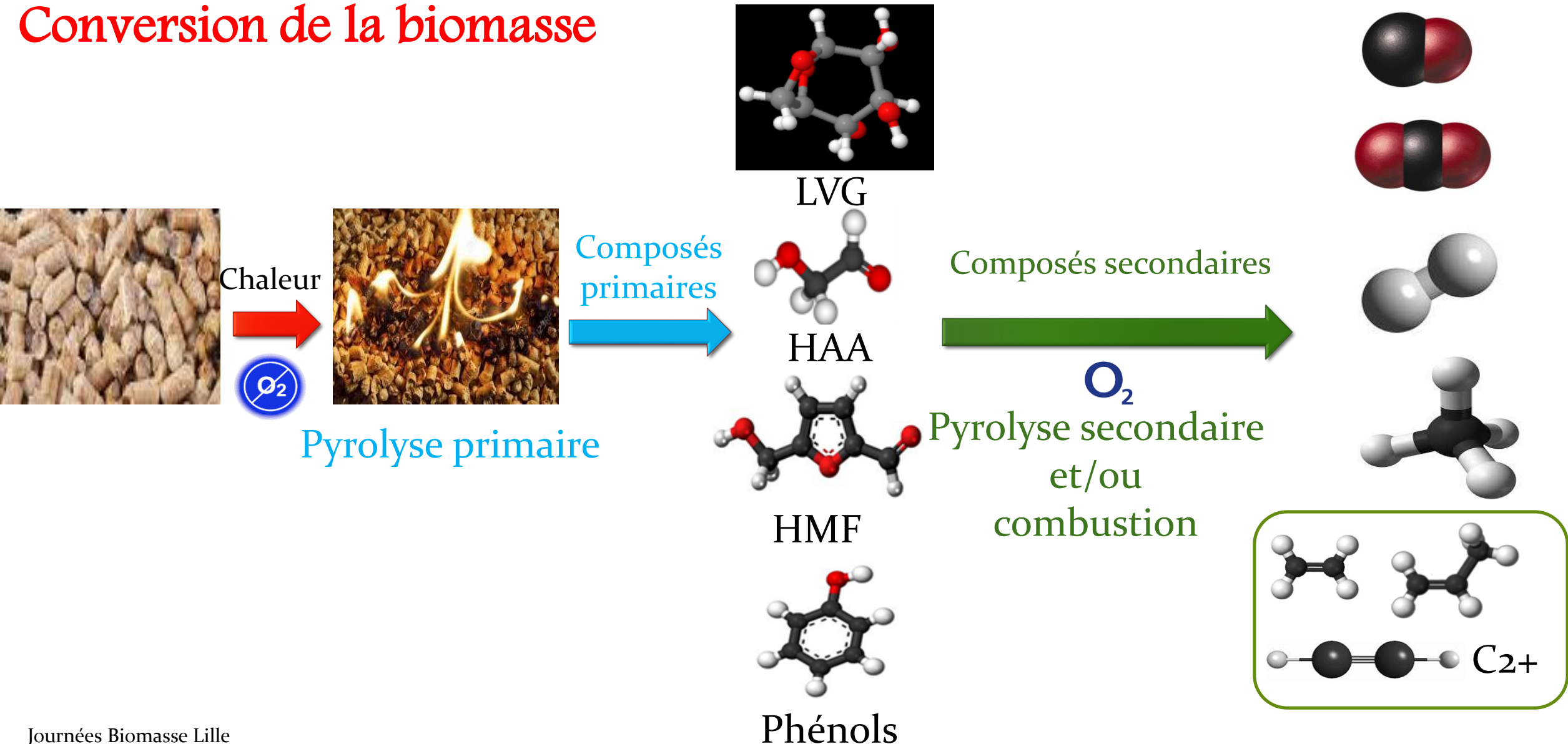
Source : ADEME



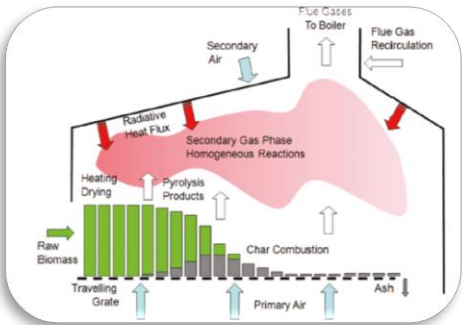
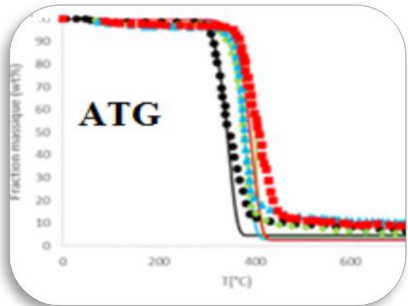
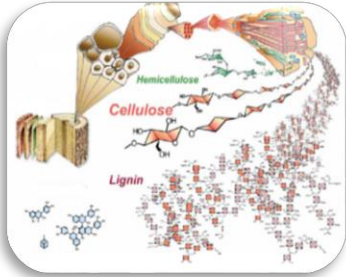


1. Introduction et contexte général

Conversion de la biomasse

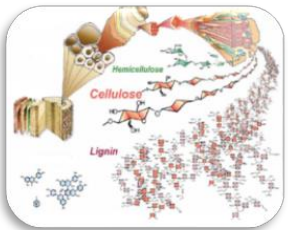


Plan

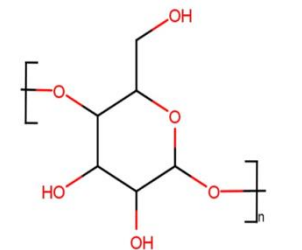
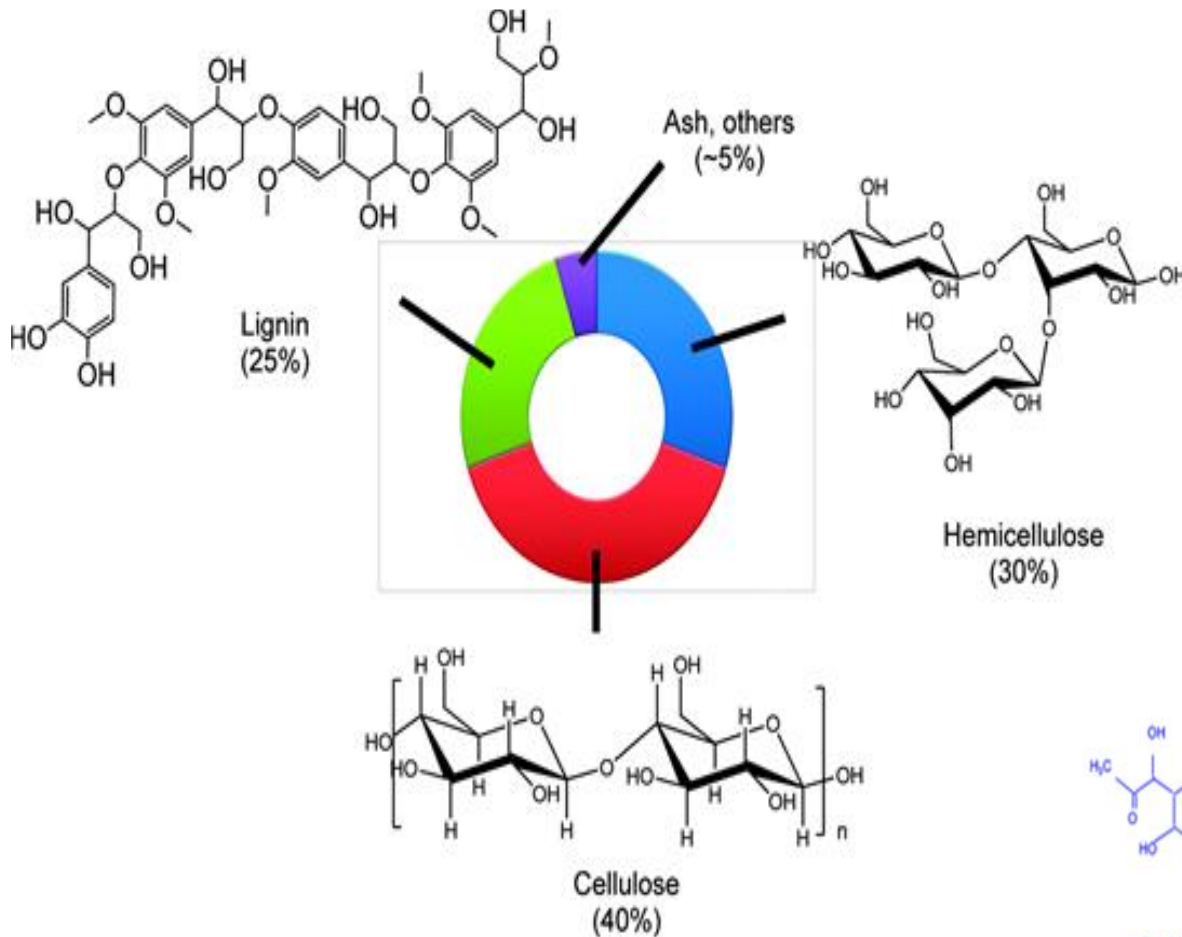


- 1- Introduction et contexte général
- 2- Démarche adoptée
- 3- Résultats
- 4- Conclusion et perspectives

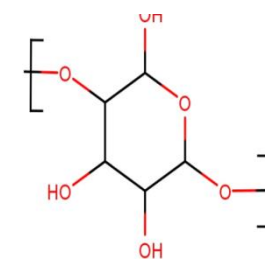
2- Démarche adoptée



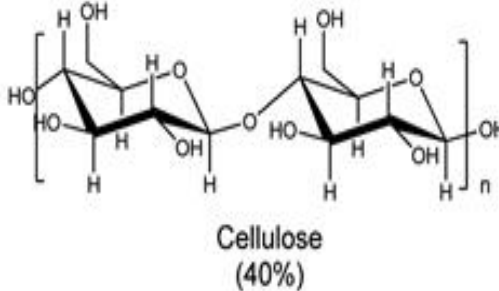
Bois



CELL : $C_6H_{10}O_5$
(44.44%C - 6.17%H - 49.38%O)



HCELL : $C_5H_8O_4$
(45.45%C 6.06%H 48.48%O)



Cellulose
(40%)



$C_{17}H_{17}O_5$
LIG-C

$C_{18}H_{17}O_5(OCH_3)_4$
LIG-O

$C_{16}H_{11}O_6(OCH_3)_4$
LIG-H

Carbone	Hydrogene	Oxygene
42-57%	5-8%	35-50%

2- Démarche adoptée



- Pyrolyse primaire et secondaire
- Combustion

Etude bibliographique

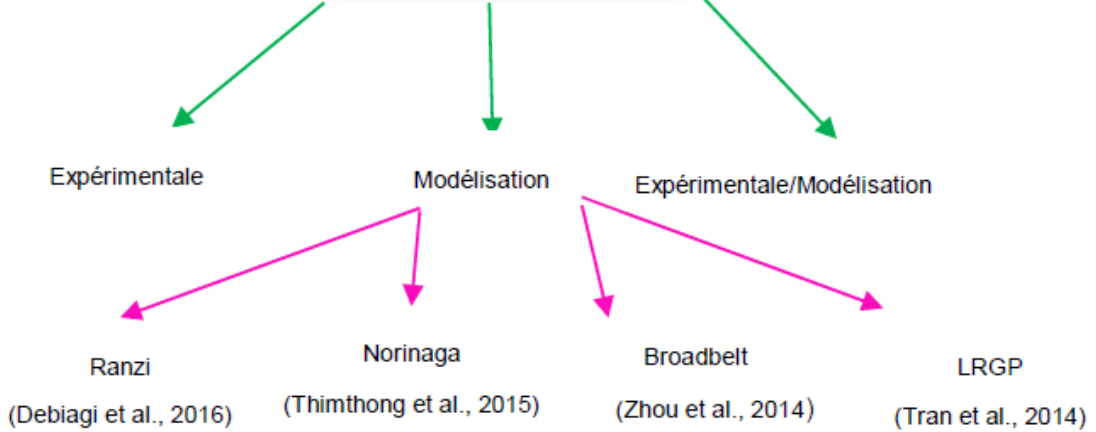
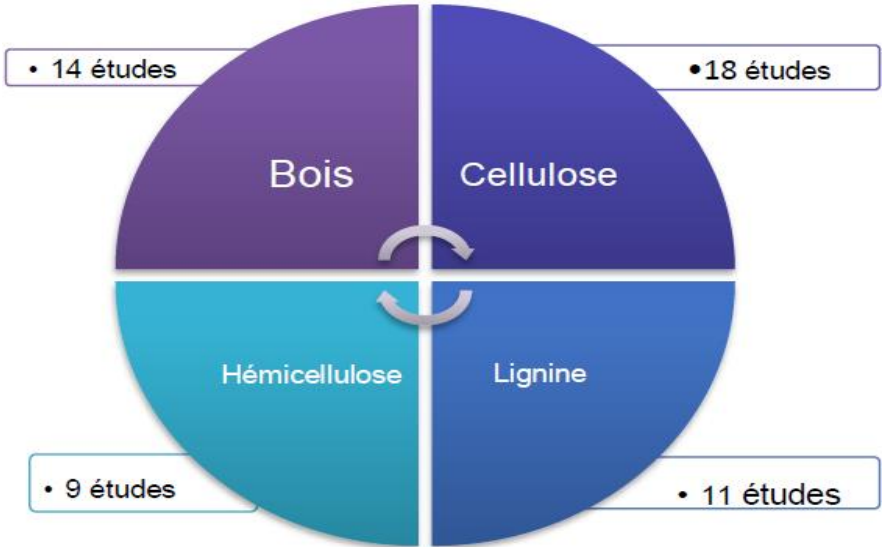
- Construction d'une base de données
- Points expérimentaux/modèles
 - Bois et ses constituants, composés clés issus de la pyrolyse primaire

- 18 cas de pyrolyse primaire,
- 12 cas de pyrolyse secondaire et/ou combustion

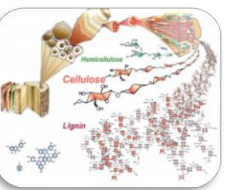
- Développement de notre propre modèle global
- Développer et valider le modèle

Benchmark

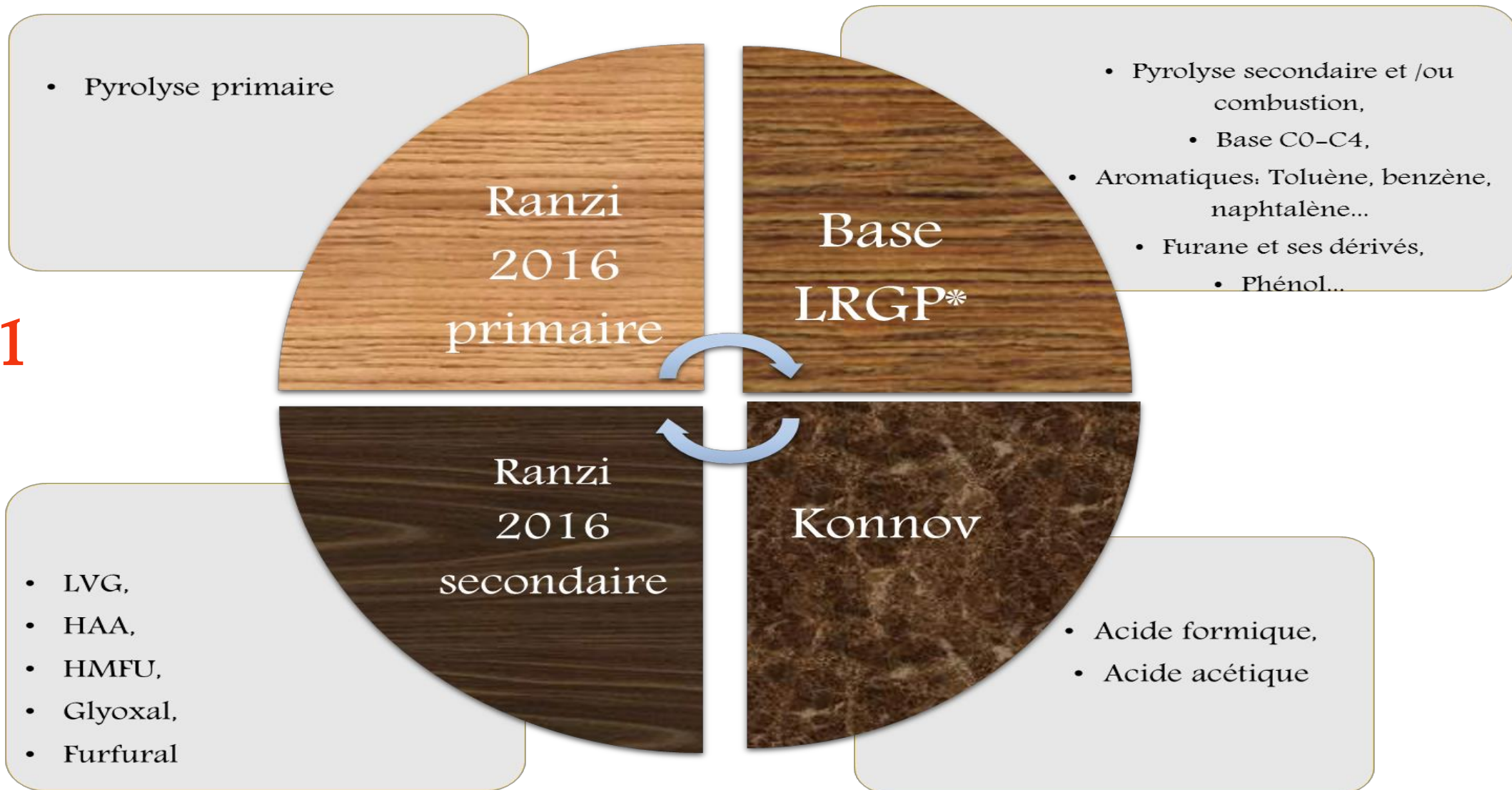
Etude



2- Démarche adoptée

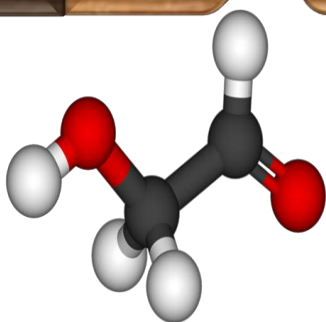
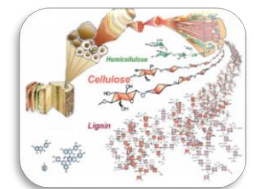


Version 1

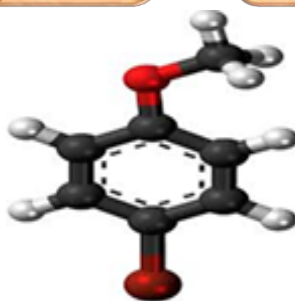


* Tran, L. S., Togbé, C., Dong, L., Felsmann, D., Oswald, P., Glaude, P. A., **Battin-Leclerc, F.**, Kohse-höinghaus, K. (2014). Combustion chemistry and flame structure of furan group biofuels using molecular-beam mass spectrometry and gas chromatography – Part II: 2-Methylfuran. Combustion and Flame, 161(3)

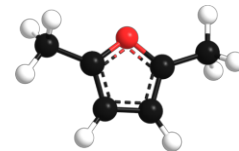
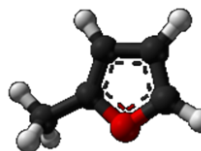
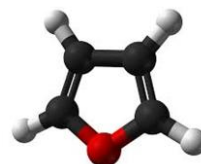
2- Démarche adoptée: Amélioration du mécanisme



HAA



Anisole

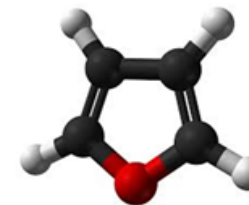
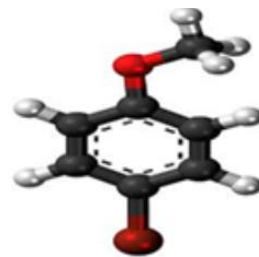
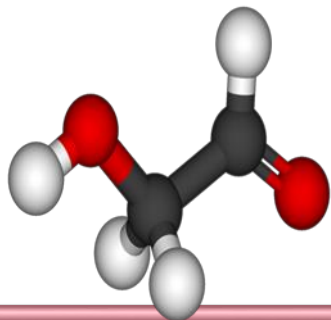
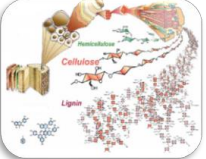


Furane, MF et DMF

Furfural

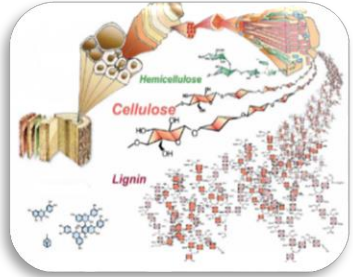
Composés
phénoliques

2- Démarche adoptée: Amélioration du mécanisme



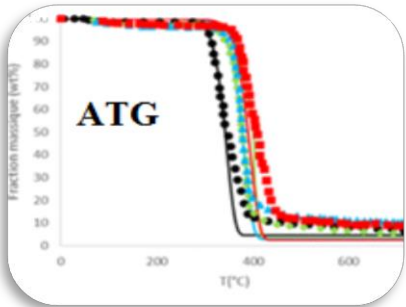


Plan

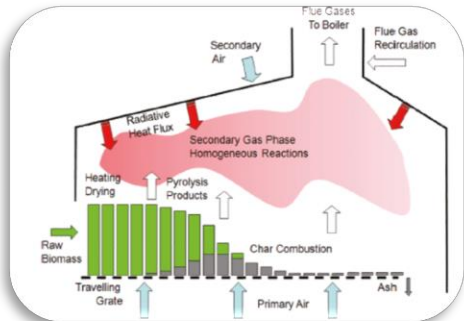


- 1- Introduction et contexte général

- 2- Démarche adoptée



- 3- Résultats



- 4- Conclusion et perspectives

3- Résultats: Mécanisme LRGP V1

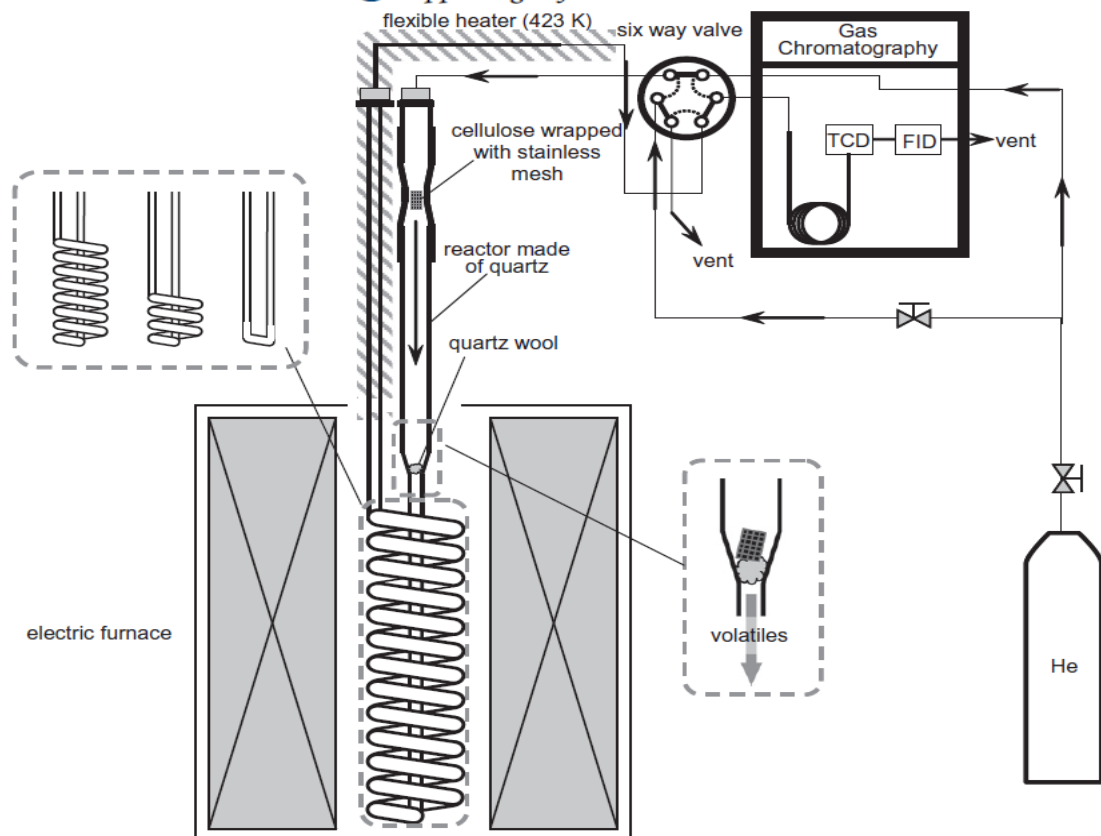


Detailed Chemical Kinetic Modeling of Vapor-Phase Reactions of Volatiles Derived from Fast Pyrolysis of Lignin

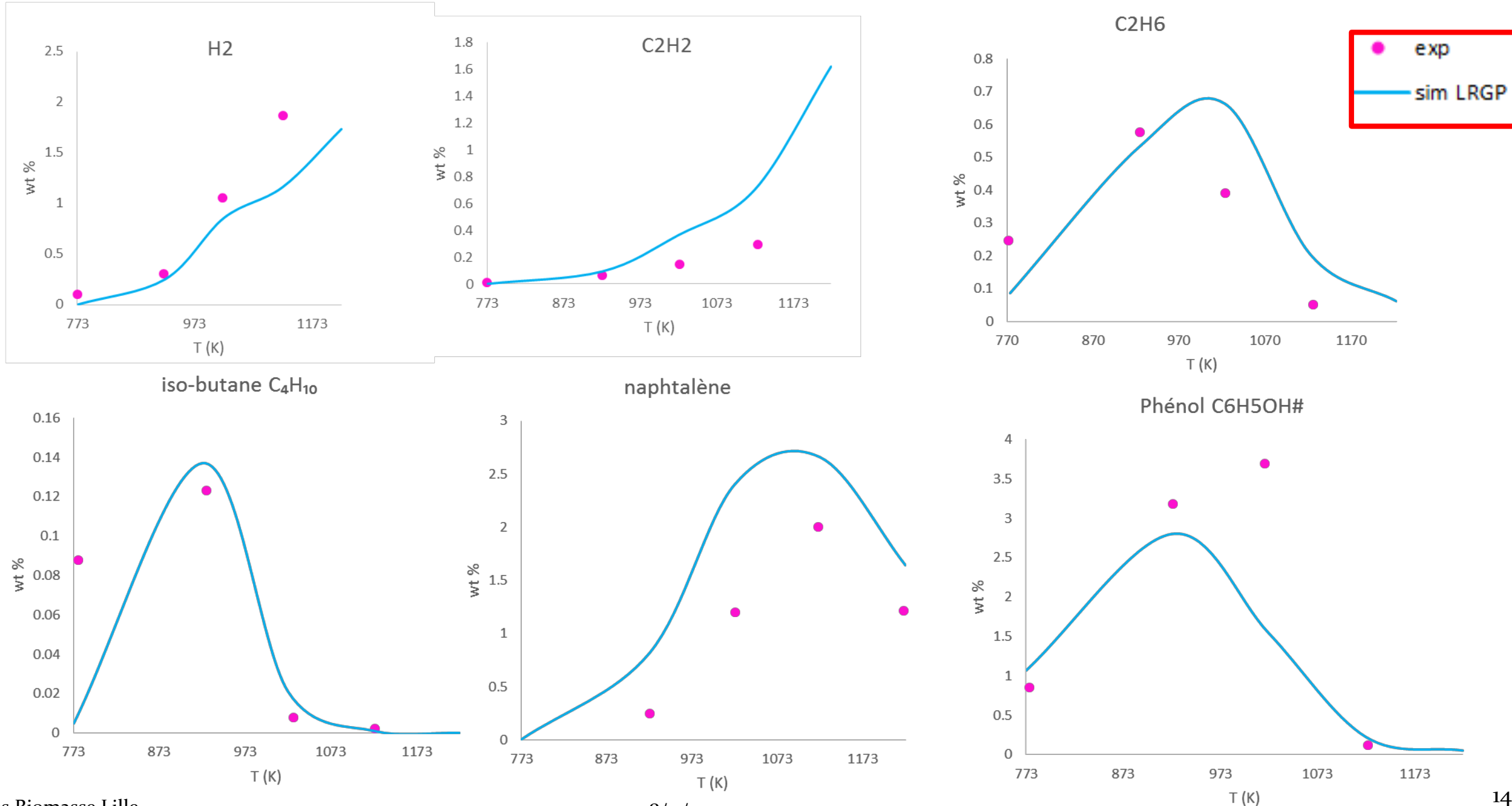
Hua-Mei Yang,[†] Srinivas Appari,[‡] Shinji Kudo,[‡] Jun-ichiro Hayashi,^{‡,§} and Koyo Norinaga^{*,‡}

[†]Interdisciplinary Graduate School of Engineering Sciences, [‡]Institute for Materials Chemistry and Engineering, and [§]Research and Education Centre of Carbon Resources, Kyushu University, Kasuga 816-8580, Japan

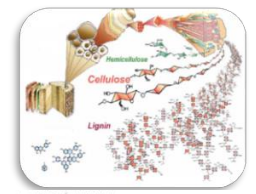
Supporting Information



	daf	
	Mole fraction	Mass fraction
CELL	0	0
HCELL	0	0
LIGC	0.48945945	0.36326399
LIGH	0.42134397	0.52845643
LIGO	0.08919658	0.10827958
ashes	0	0
water	0	0
	1	1



3- Résultats: Mécanisme LRGP V2: HAA



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Fuel 80 (2001) 1697-1709



www.fuelfirst.com

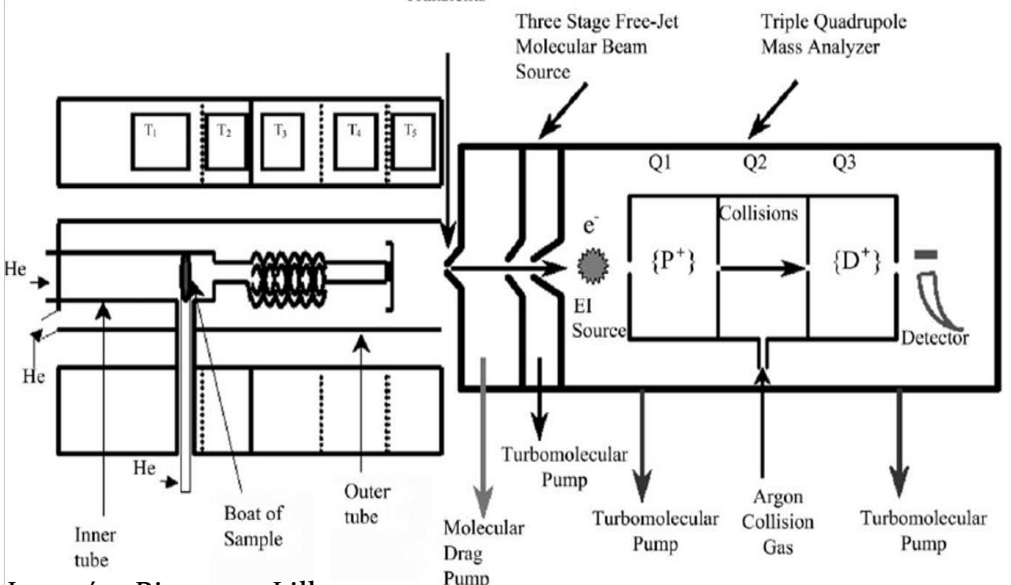
Kinetic analysis of the gas-phase pyrolysis of carbohydrates

Eun-Jae Shin^a, Mark R. Nimlos^{a,b}, Robert J. Evans^{a,*}

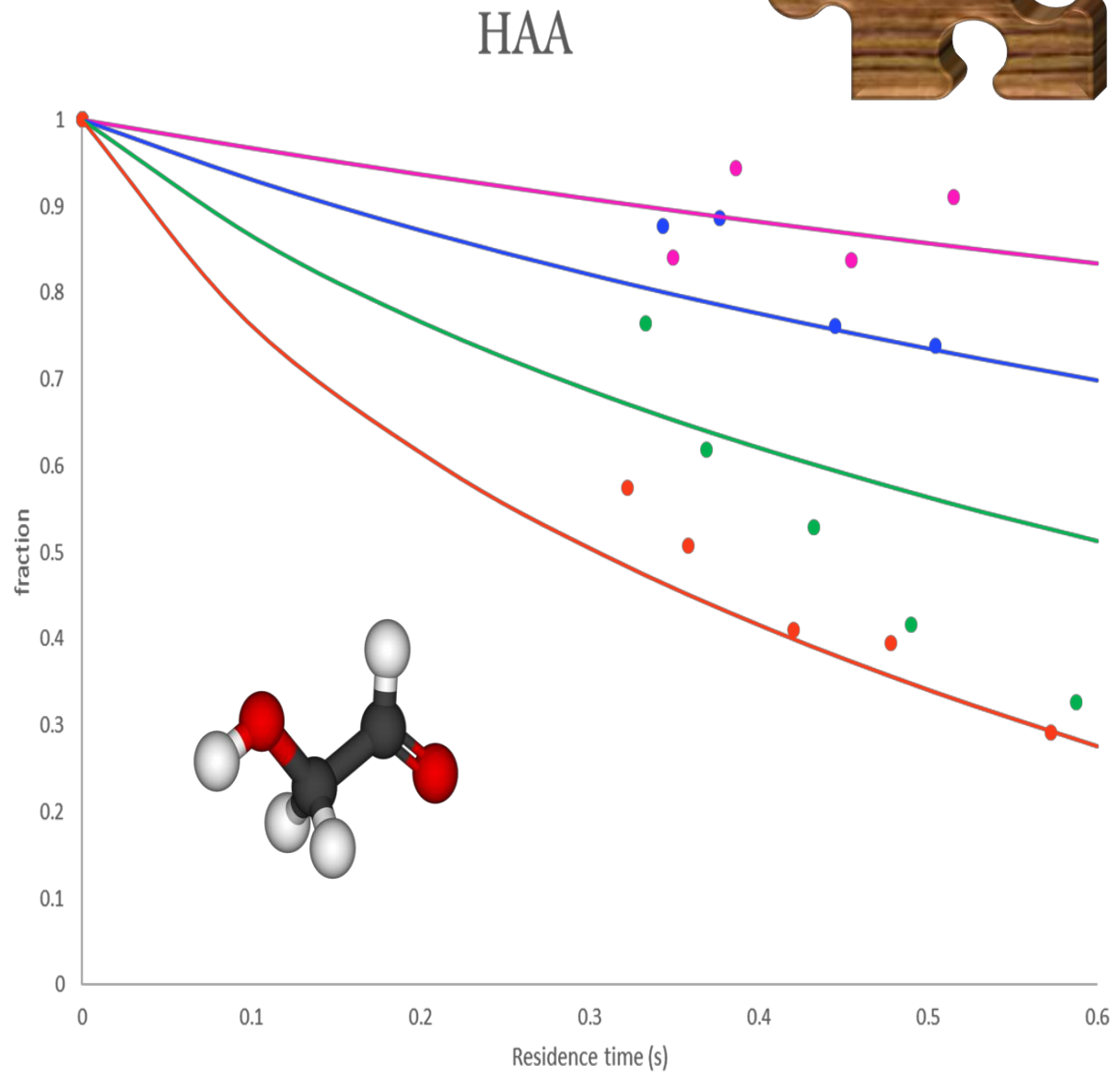
^aNational Renewable Energy Laboratory, 1617 Cole Blvd., Golden, CO 80401, USA

^bDepartment of Chemical Engineering, Colorado School of Mines, Golden, CO 80401, USA

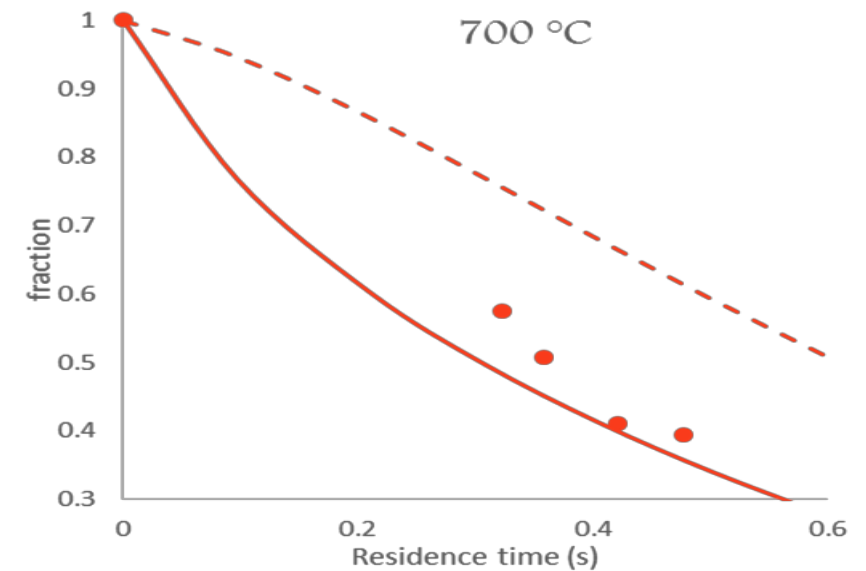
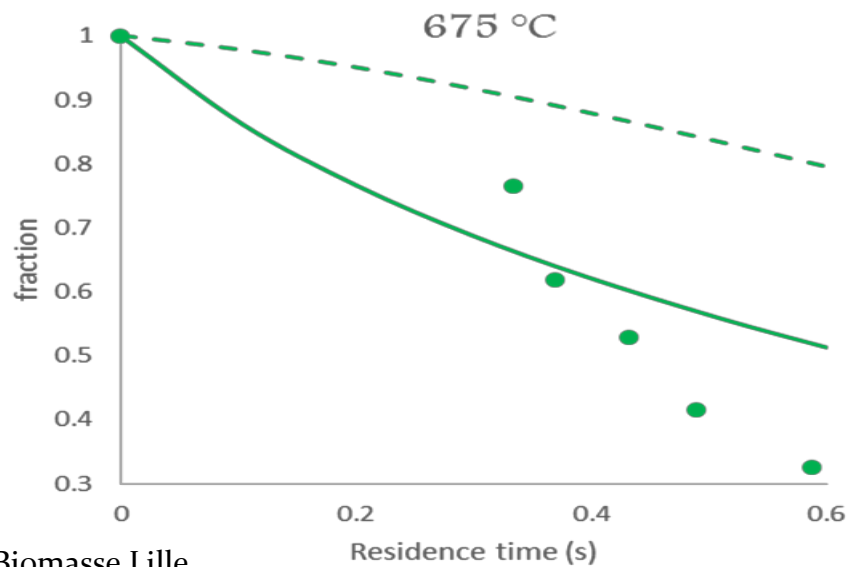
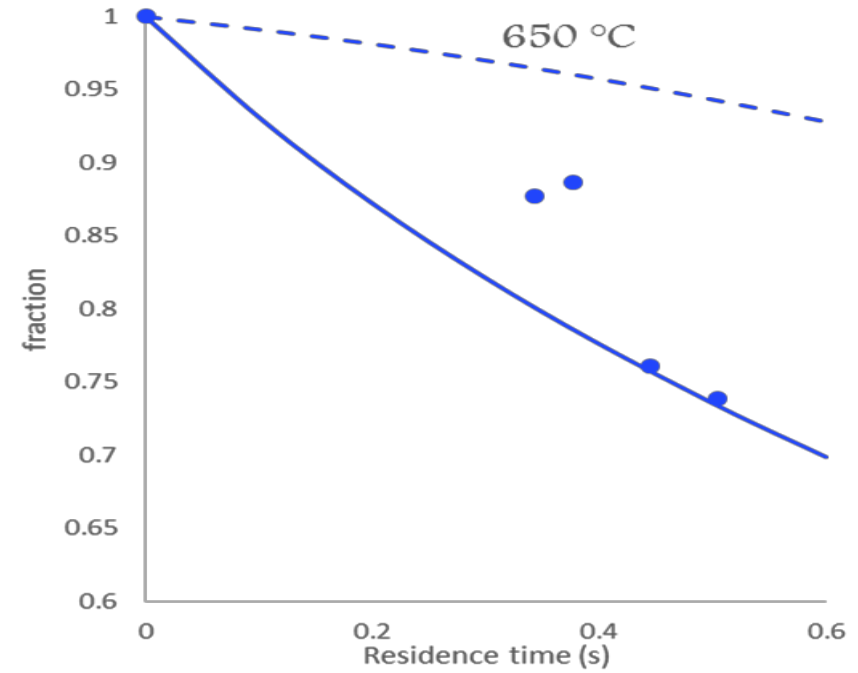
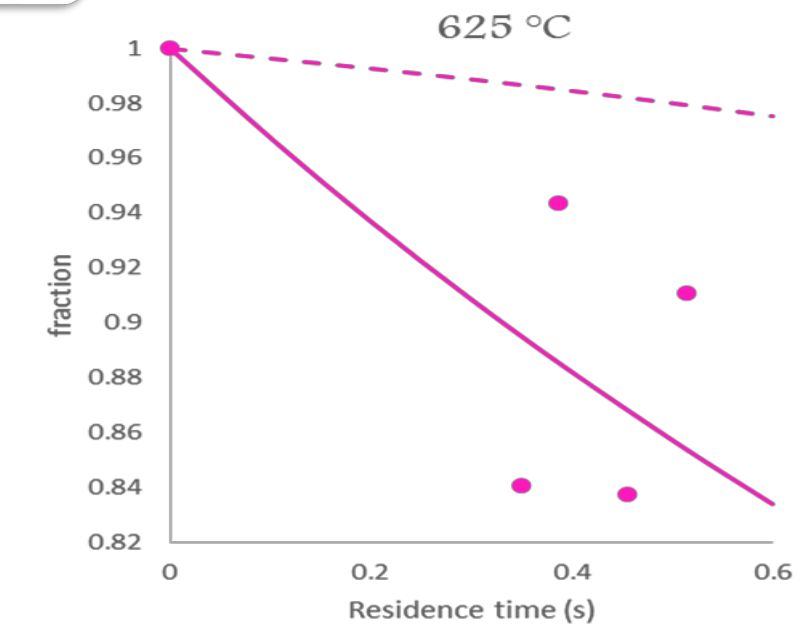
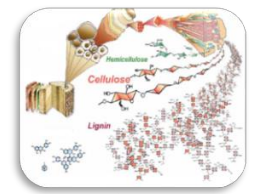
Received 15 June 2000; revised 5 January 2001; accepted 29 January 2001



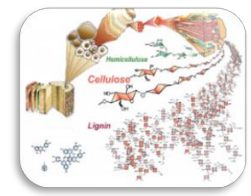
- exp 625 C
- exp 650 C
- exp 675 C
- exp 700 C
- sim 625 C
- sim 650 C
- sim 675 C
- sim 700 C



3- Résultats: Mécanisme LRGP V2: HAA



3- Résultats: Mécanisme LRGP V3: Anisole



Contents lists available at [ScienceDirect](#)

Combustion and Flame

journal homepage: www.elsevier.com/locate/combustflame



Detailed kinetic study of anisole pyrolysis and oxidation to understand tar formation during biomass combustion and gasification



Milena Nowakowska, Olivier Herbinet, Anthony Dufour, Pierre-Alexandre Glaude *

Laboratoire Réactions et Génie des Procédés (LRGP), CNRS, Université de Lorraine, ENSIC, 1 rue Grandville, 54000 Nancy, France



$P=800$ torr

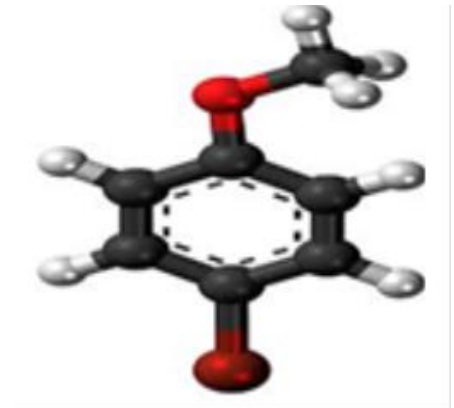
$T=673-1173$ K

$\tau=2$ sec

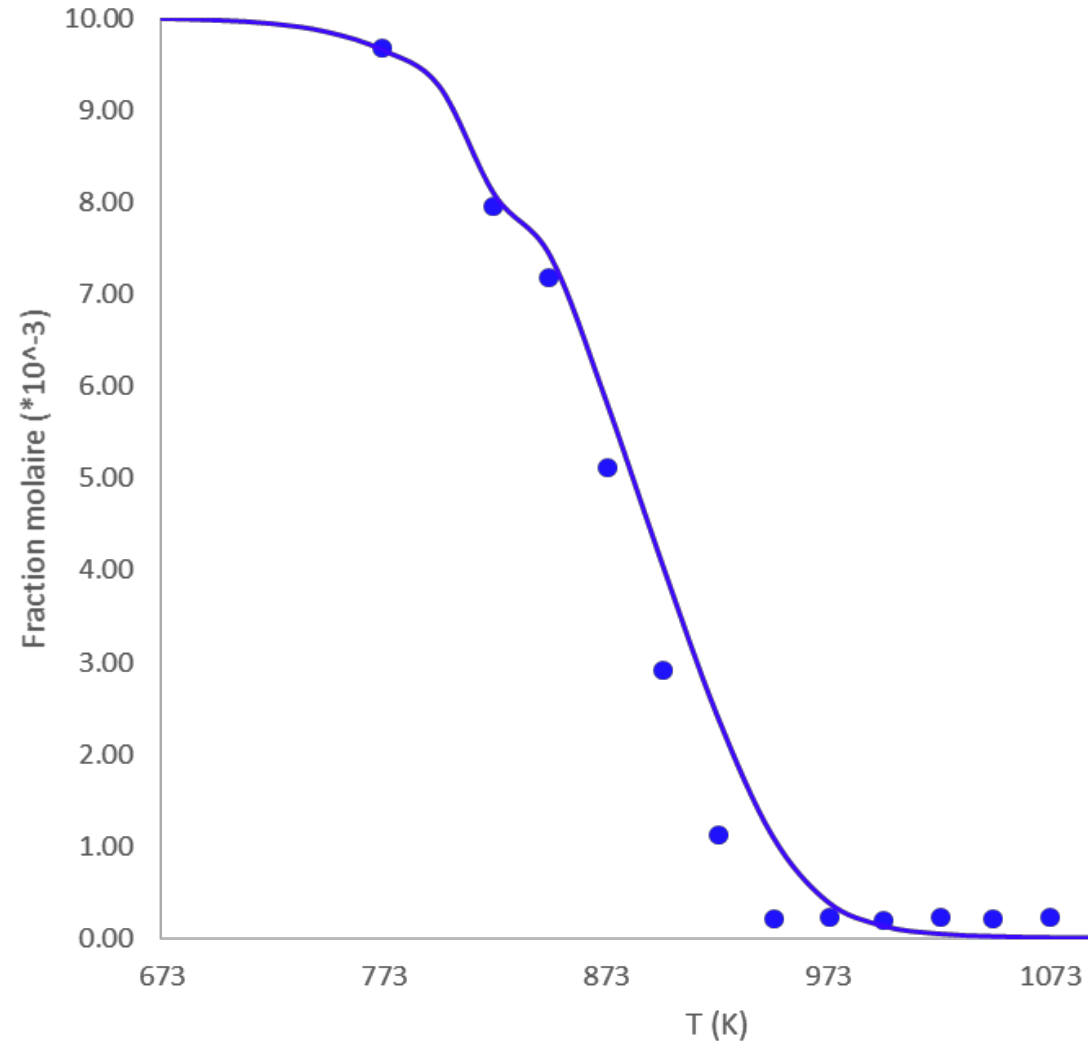
Pyrolyse et oxydation stœchiométrique

$X_{\text{anisole}}=0,01$ (pour la pyrolyse)

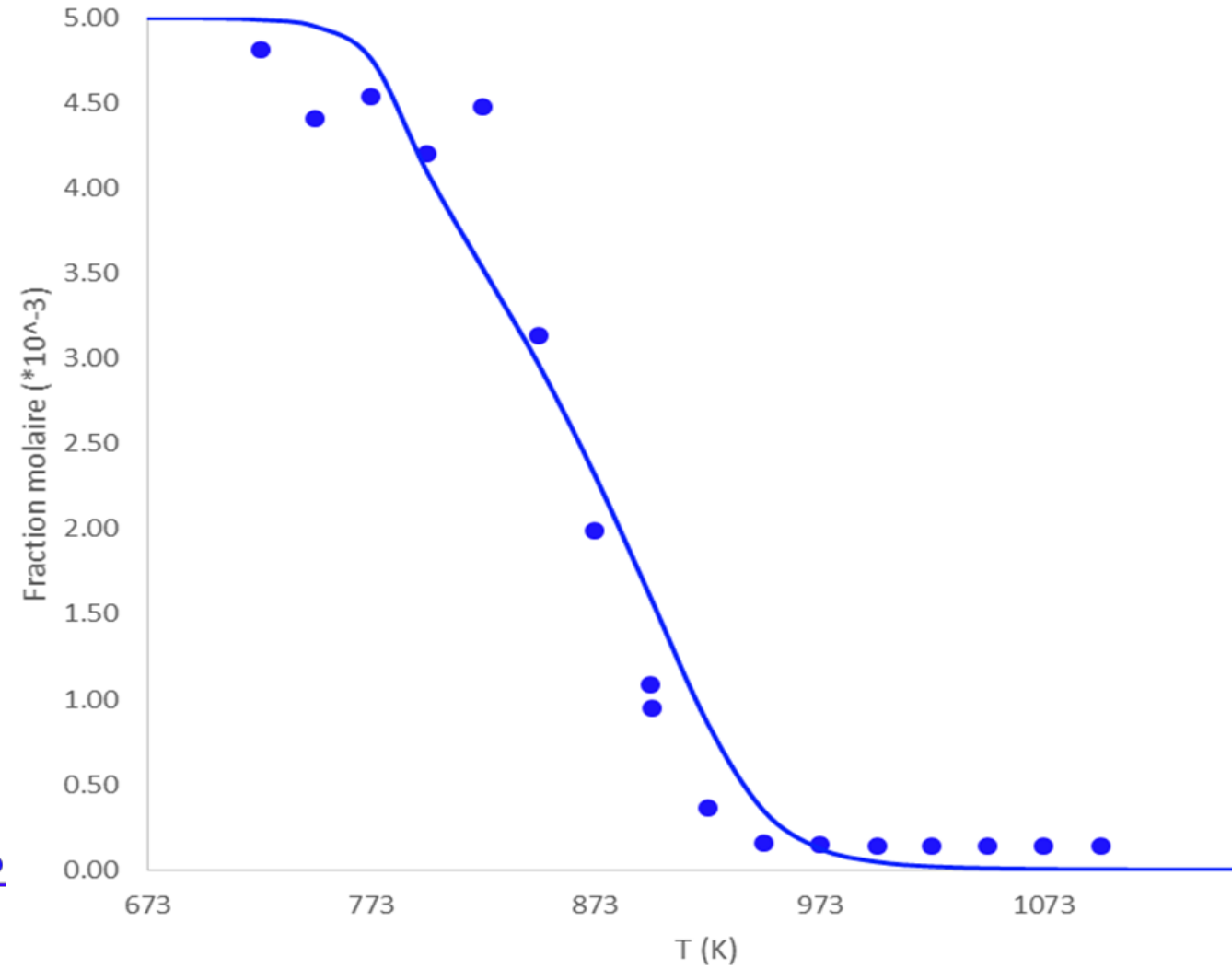
$X_{\text{anisole}}=0,005$ (pour l'oxydation stœchiométrique)



Pyrolyse de l'anisole

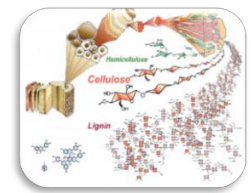


oxydation stoechiométrique de l'anisole-LRGP V3



● exp
— sim LRGP V3

3- Résultats: Mécanisme LRGP V4: Furane et ses dérivés



Combustion and Flame 181 (2017) 251–269

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Combustion and Flame

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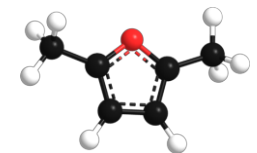
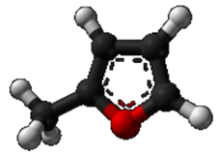
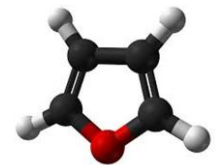
Comparative experimental and modeling study of the low- to moderate-temperature oxidation chemistry of 2,5-dimethylfuran, 2-methylfuran, and furan

Luc-Sy Tran^{a,*}, Zhandong Wang^{a,1}, Hans-Heinrich Carstensen^b, Christian Hemken^a, Frédérique Battin-Leclerc^c, Katharina Kohse-Höinghaus^{a,*}

^a Department of Chemistry, Bielefeld University, Universitätsstraße 25, D-33615 Bielefeld, Germany

^b Laboratory for Chemical Technology (LCT), Ghent University, Technologiepark 914, 9052 Ghent, Belgium

^c Laboratoire Réactions et Génie des Procédés, UMR 7274 CNRS - Université de Lorraine, 1 rue Grandville, 54000 Nancy, France

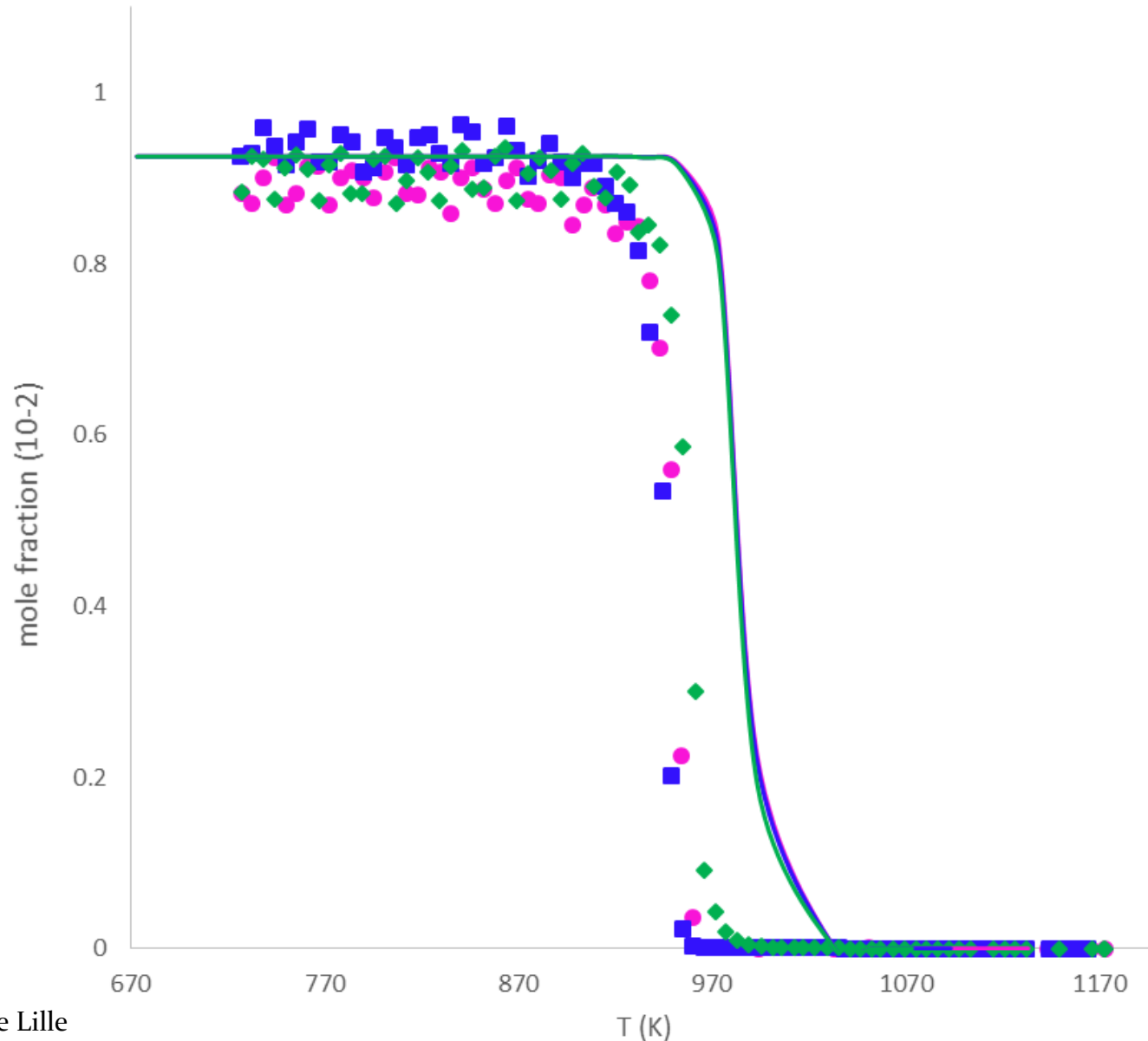


Experimental conditions.

	Name of mixture	ϕ	Gas flow rate (SLM) (std. conditions: 273.15 K, 1 atm)				P (bar)
			Total	Ar	O ₂	Fuel	
Furan oxidation	F0.5	0.46	0.9993	0.900	0.090	0.0093	1.0
	F1.0	0.92	0.9993	0.945	0.045	0.0093	1.0
	F2.0	1.85	0.9993	0.968	0.023	0.0093	1.0
MF oxidation	MF0.5	0.50	1.0000	0.870	0.120	0.0100	1.0
	MF1.0	1.00	1.0000	0.930	0.060	0.0100	1.0
	MF2.0	2.00	1.0000	0.960	0.030	0.0100	1.0
DMF oxidation	DMF0.5	0.53	1.0005	0.840	0.150	0.0105	1.0
	DMF1.0	1.05	1.0005	0.915	0.075	0.0105	1.0
	DMF2.0	2.10	1.0005	0.953	0.038	0.0105	1.0

3- Résultats: Mécanisme LRGP V4: Furane et ses dérivés

Furan-LRGP V4



● exp $\phi = 0.5$

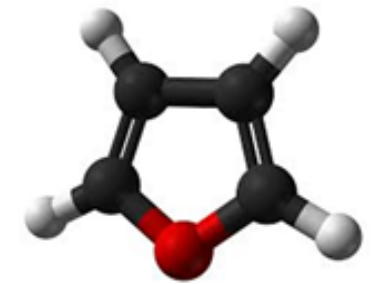
■ exp $\phi = 1$

◆ exp $\phi = 2$

— sim LRGP V4 $\phi = 0.5$

— sim LRGP V4 $\phi = 1$

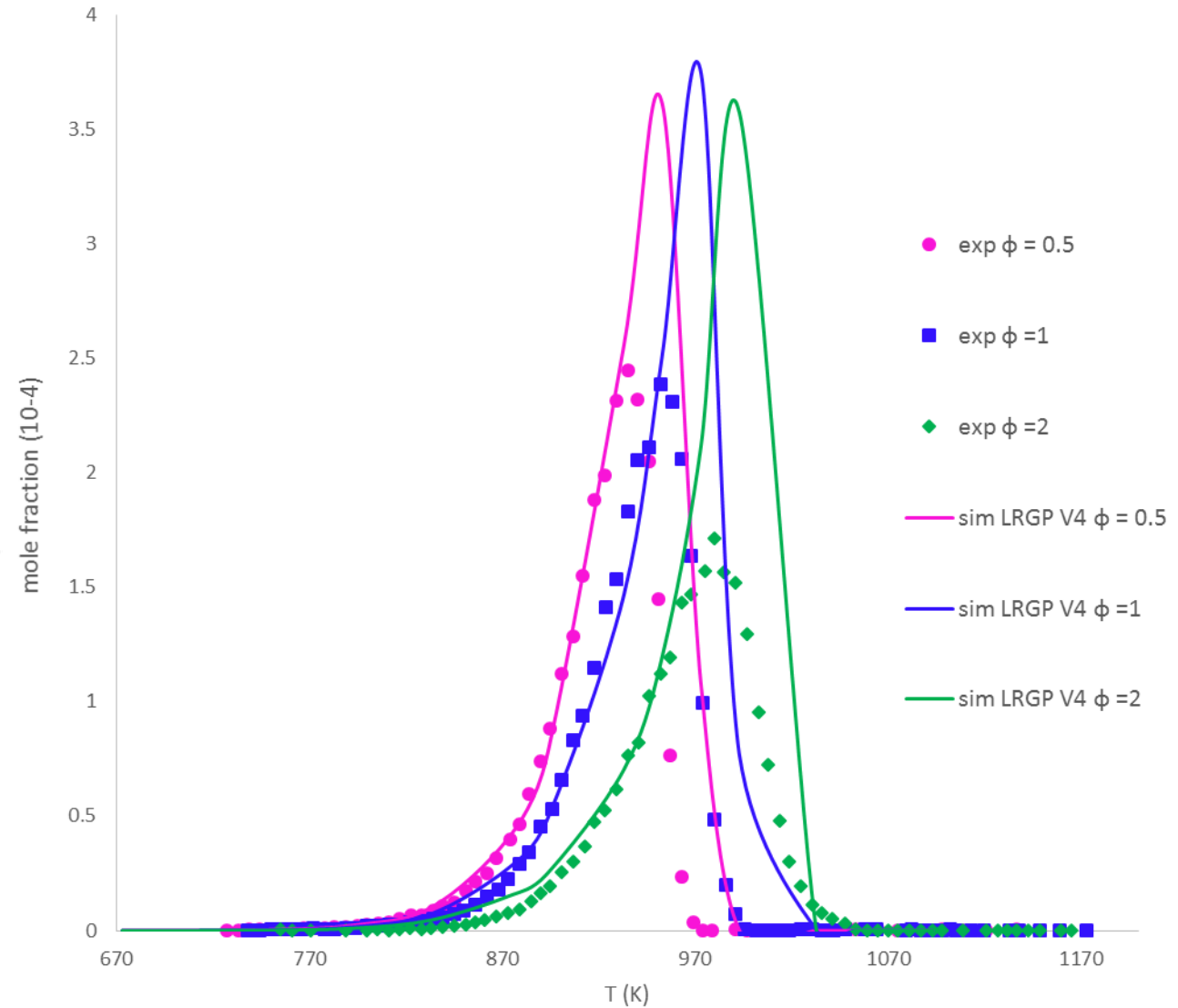
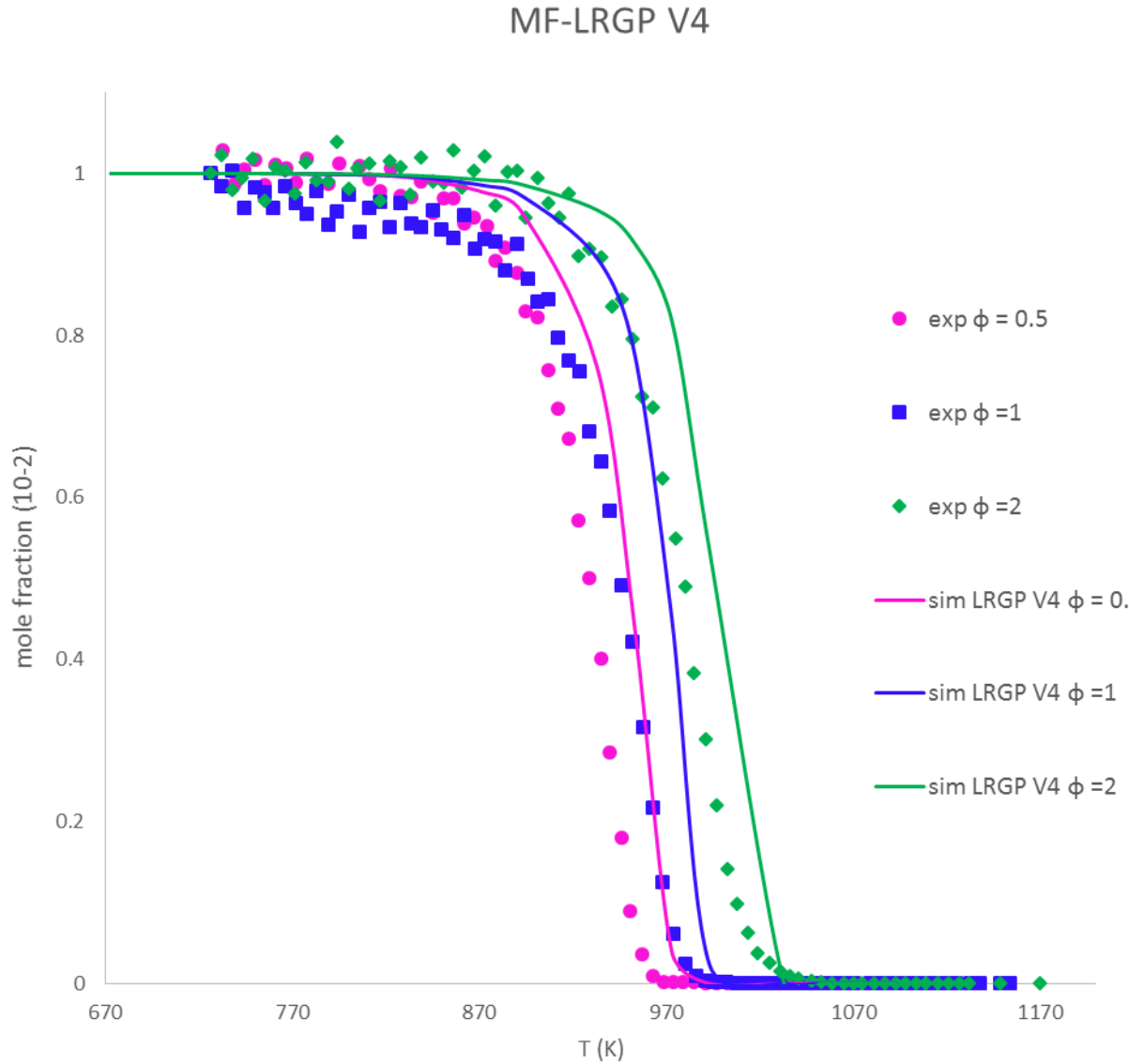
— sim LRGP V4 $\phi = 2$



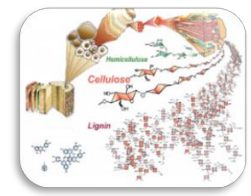
3- Résultats: Mécanisme LRGP V4: Furane et ses dérivés



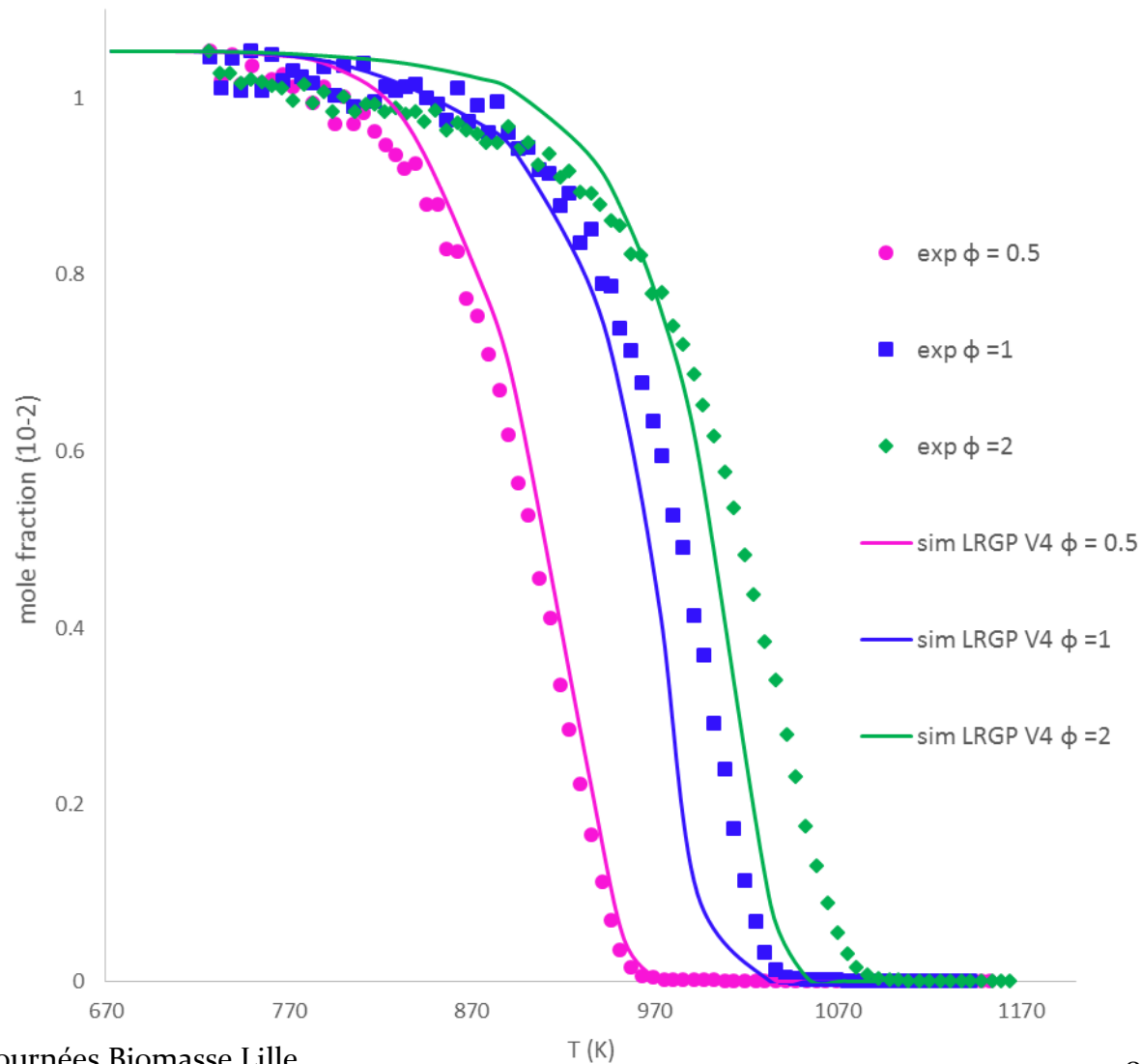
MF oxidation: furfural (furylCHO)-LRGP V4



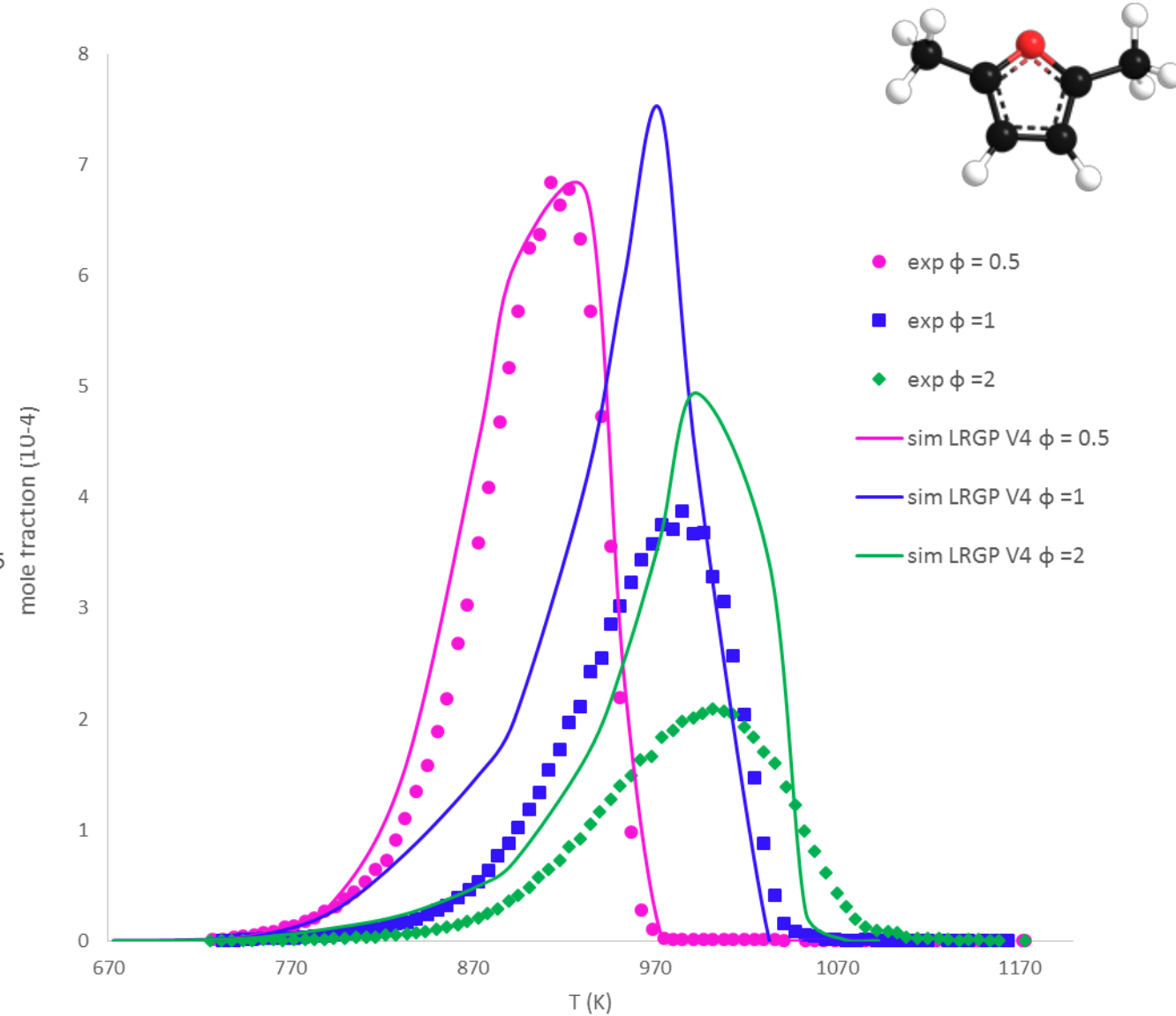
3- Résultats: Mécanisme LRGP V4: Furane et ses dérivés



DMF-LRGP V4

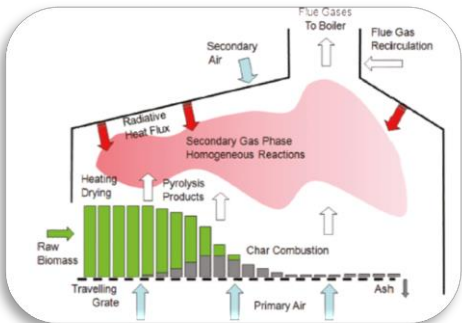
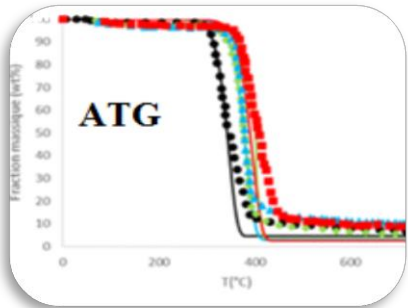
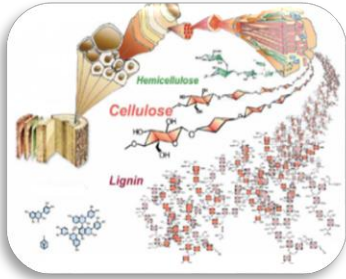


DMF oxidation: 5-methylfurfural (MF-CHO)-LRGP V4



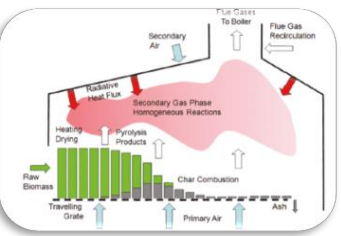


Plan

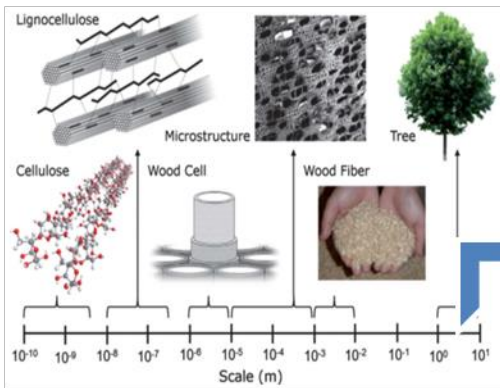


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- 3- Résultats
- 4- Conclusion et perspectives

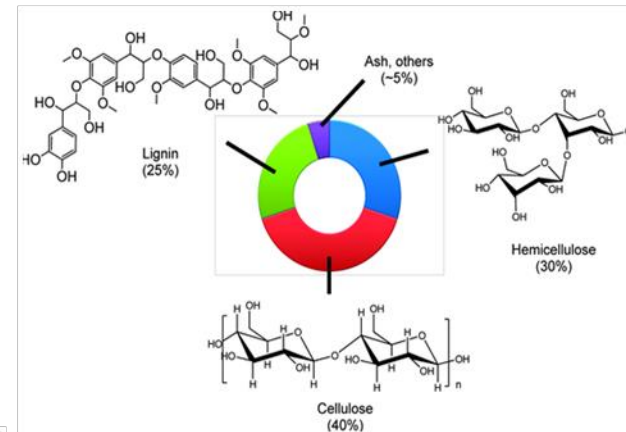
4- Conclusion et perspectives



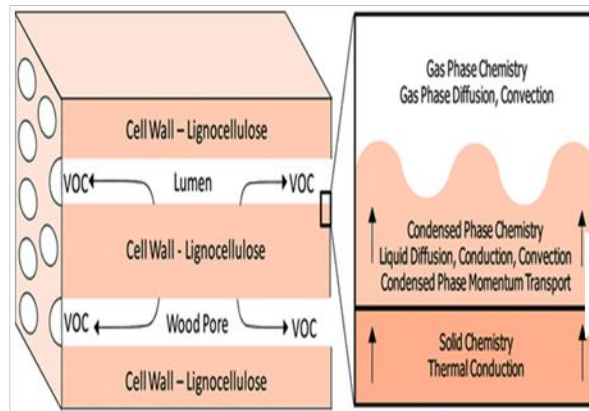
L'étude de la décomposition thermique de la biomasse, en général et du bois en particulier, présente plusieurs difficultés:



Multi-
échelle

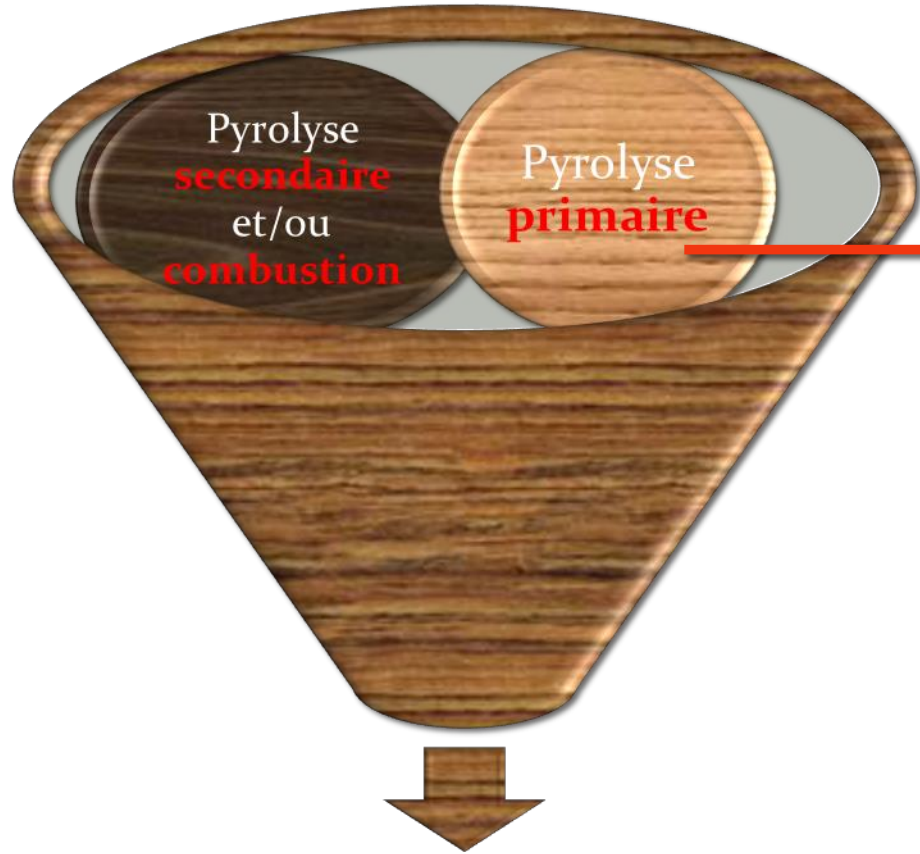
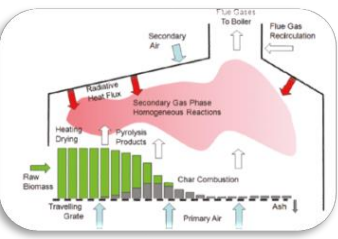


Multi-
composés



Multi-
phase

4- Conclusion et perspectives

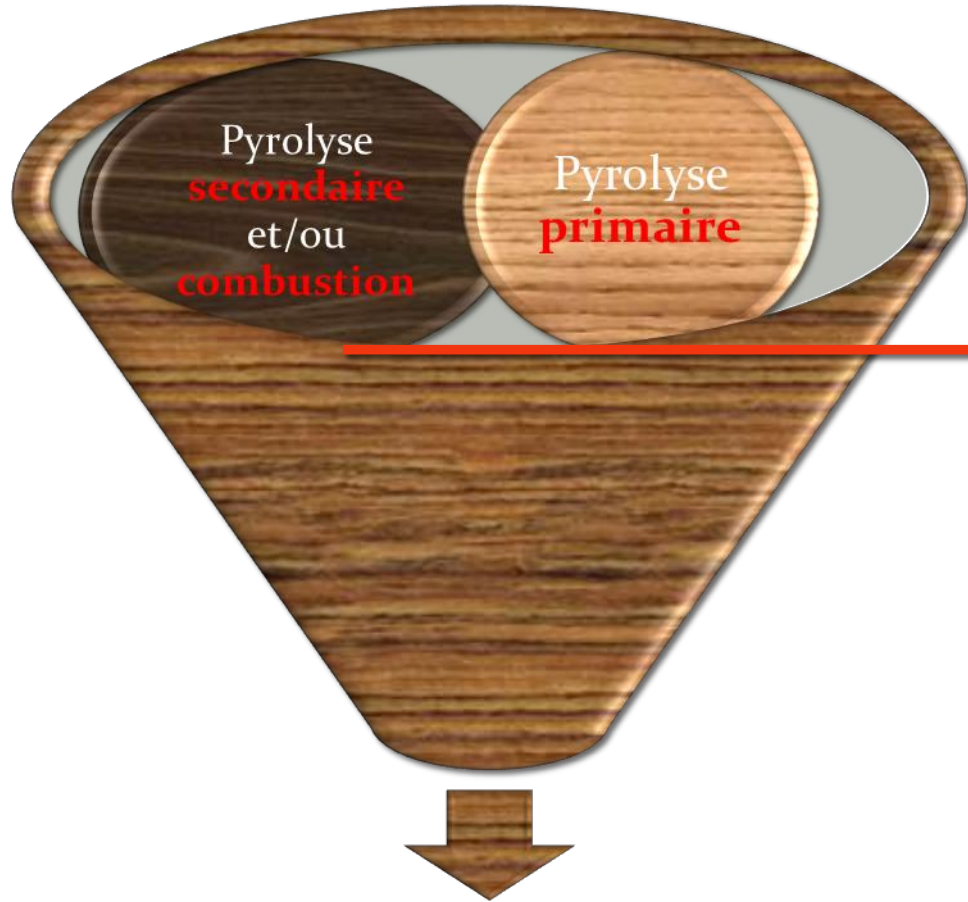
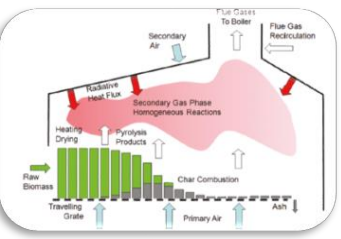


Modèle cinétique global

A optimiser sur un grand set de points expérimentaux (résultats de *benchmark primaire*)

Etude	Procédé	Type de réacteurs	Composé étudié	Température	vitesse de chauffe
Pyrolyse primaire					
Jakab et al. , 1995	ATG sous Argon	_____	6 types de lignine	T= 200-900 °C	20 °C/min
Paul T et al. , 1996	ATG sous Azote	Batch statique	Bois de pin Cellulose Hémicellulose Lignine	Tfinale=300, 420, 600 ou 720 °C	5, 20, 40 ou 80 K/min
Aho et al. , 2008	ATG sous azote/Pyrolyse	Lit fluidisé	Bois de pin Cellulose Hémicellulose	Tracteur: jusqu'à 460 °C	ATG: 20°C/min Pyrolyse: 5 °C/min
Corbetta et al. , 2014	DTG sous azote/Pyrolyse	Tubulaire	Bois de peuplier	* DTG: 0-500 °C *Pyrolyse: 368 ° C et 470 ° C	DTG: 10°C/min
Werner et al. , 2014	ATG/DTG sous azote	_____	Cellulose Hémicellulose	Tf= 600 °C	10°C/min
Le Brech et al. , 2015	ATG sous Argon/Pyrolyse	Lit fixe en quartz en forme de U vertical	Miscanthus Douglas Chêne	Tracteur: jusqu'à 500 °C	5 °C/min
Le Brech et al. , 2016	ATG sous Argon/Pyrolyse	Lit fixe en quartz en forme de U vertical	MiscanthusxGiganteus Cellulose Lignine Holocellulose	Tracteur: jusqu'à 500 °C	5°C/min
Chen et al. , 2016	ATG sous azote/Pyrolyse	Lit fixe	Sciure de bois de peuplier	Tracteur 400, 450, 500, 550 et 600 °C	10, 30 et 50 °C / min

4- Conclusion et perspectives

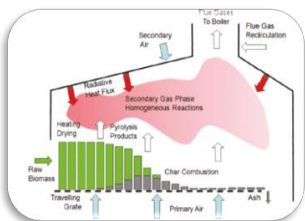


Modèle cinétique global

Ajout du sous-mécanisme de décomposition de furfural et de composés phénoliques: *LRGP V5* et *LRGP V6*

Validation de modèle cinétique global.

4- Conclusion et perspectives





Merci pour votre attention.
Des questions?