

Multi-scale simulation of fluidized bed biomass gasification

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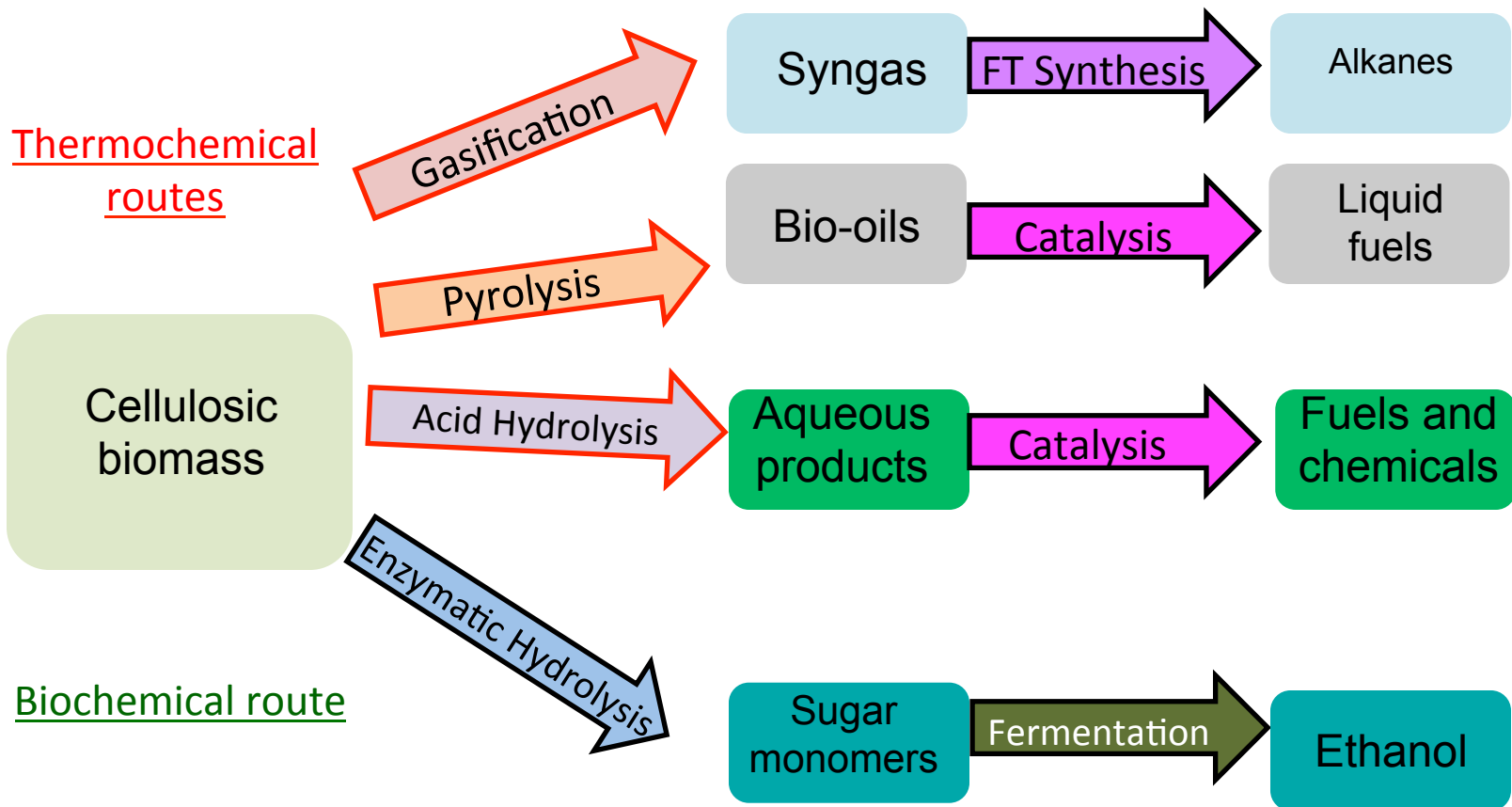
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NETL Workshop of Multiphase Simulations

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Project support by BP

Biomass to liquids pathways



- Gasification offers improved feedstock utilization versus existing 1st generation routes
- Gasification allows production of drop-in fuels (e.g. FT Diesel) as well as chemicals

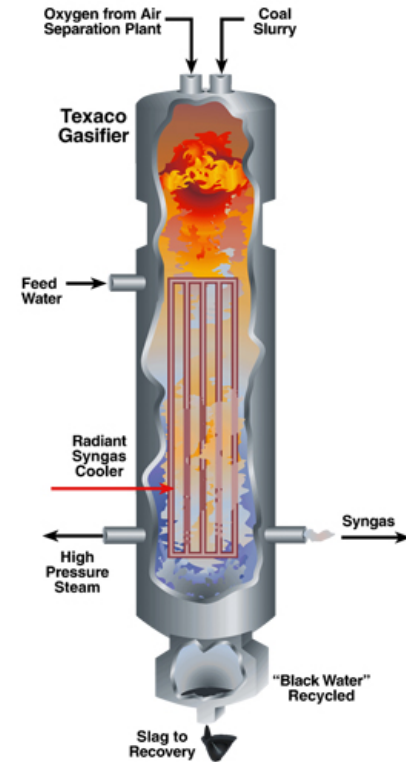
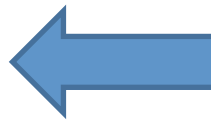
Fluidized bed gasification of biomass

Raw biomass characteristics

- High moisture content
- Expensive particle size reduction



Not suitable for raw biomass, unless it is pre-torrefied, see Bates and Ghoniem, Bioresource Tech



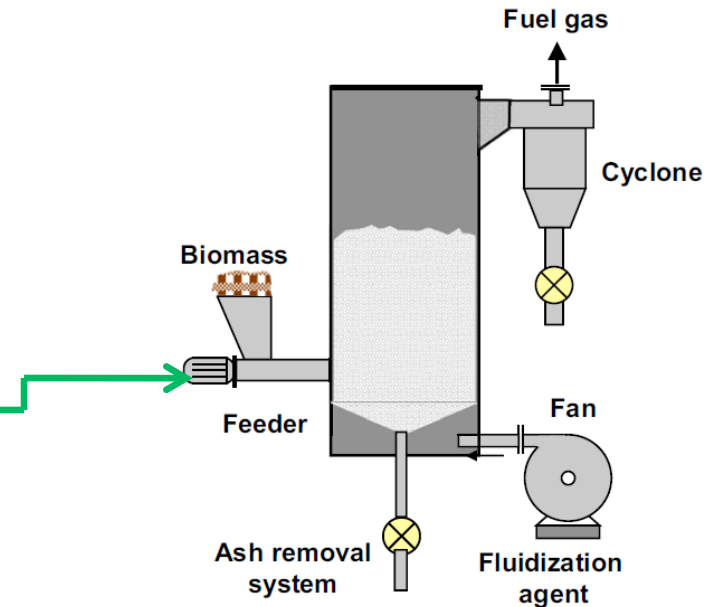
Entrained flow gasifier: Very dilute particle-gas multiphase flow

- High operating temperatures
- High levels of carbon conversion with low tar content
- Requires very fine particles (<mm)

Fluidized bed gasification of biomass

Raw biomass characteristics

- High moisture content
- Expensive particle size reduction



Fluidized bed: Widely used paradigm for dense particle-gas multiphase flows

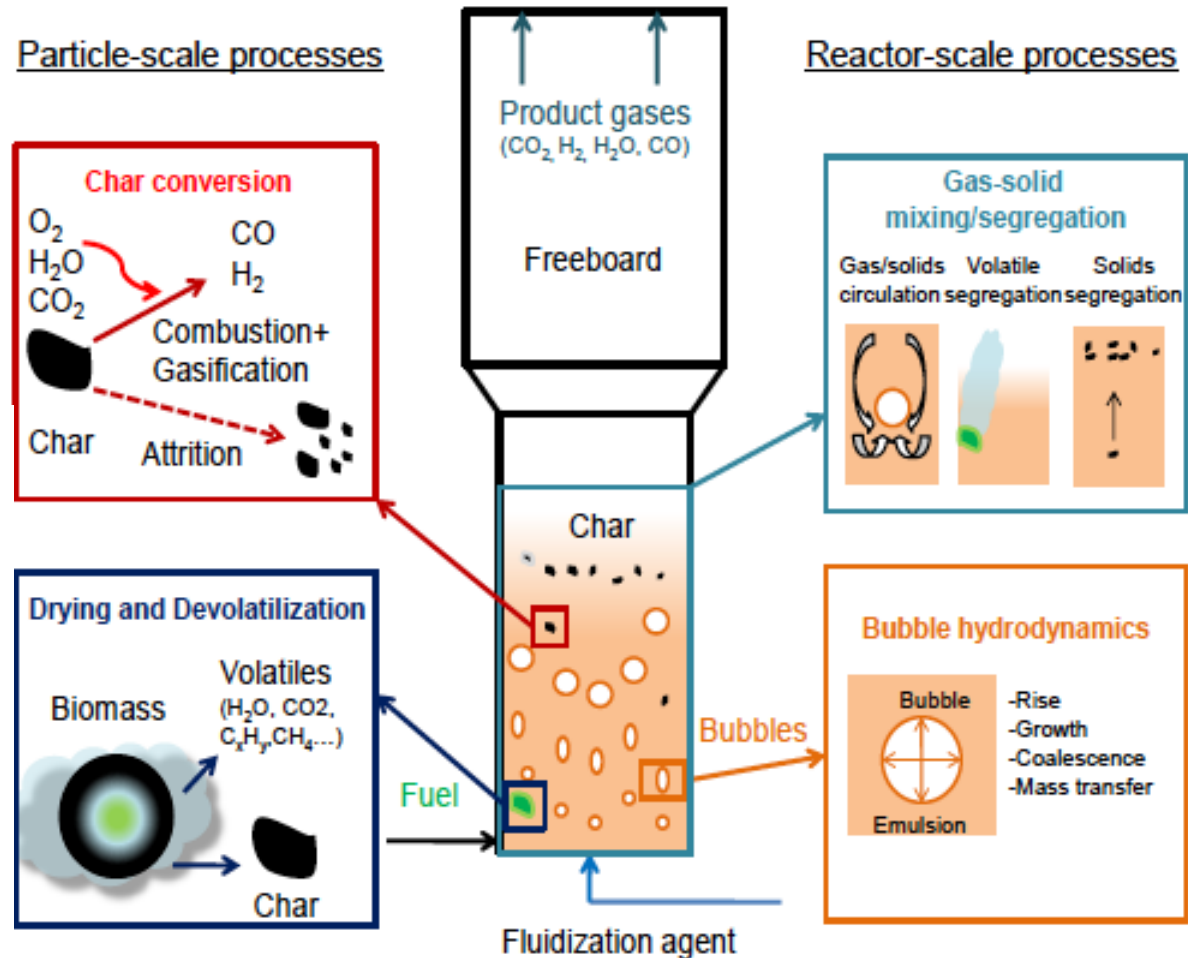
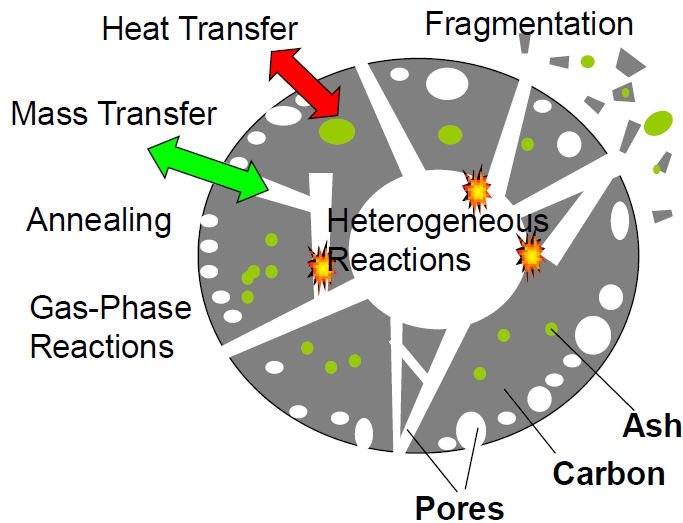
- High surface area contact between fluid and solid per unit bed volume
- High levels of intermixing
- Suitable for coarse particles with large residence times
- Lower levels of carbon conversion with considerable tar content

Appropriate for biomass gasification, poses operational and modeling challenges

Multi-scale nature of biomass gasification

Multi-scale process:

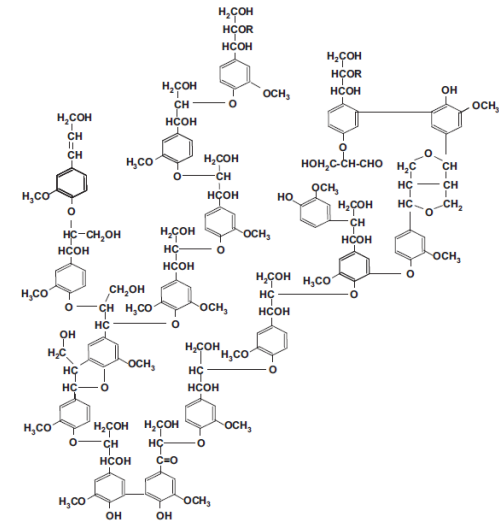
- Gas-phase chemistry
- Surface chemistry
- Single-particle modeling
- Hydrodynamics
- Mixing - Segregation



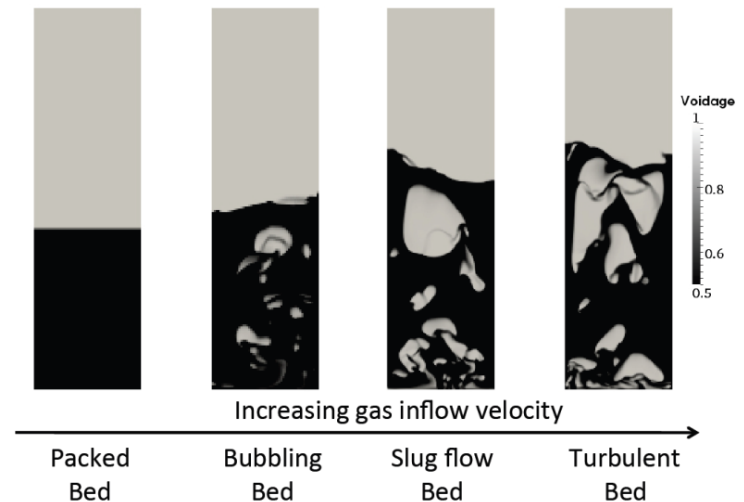
Fluidized bed biomass gasification Modeling

Challenges

- Complex interplay between:
 - Multiphase fluid dynamics
 - Massive chemical reaction networks
- Existing chemical kinetic mechanisms are too computationally demanding
 - Ranzi et al. [2] 460 species, 16000 reactions
 - Reliable chemistry reduction strategies are needed
- Simulating industrial scale reactors requires the development of advanced closure sub-models for the physics description



Typical structure of softwood lignin
(Faravelli et al., 2010 [2])



Multiscale simulations & technical challenges

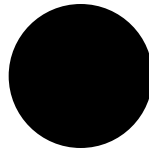
Technical challenges in fluidized bed gasification

1. Expensive scale-up

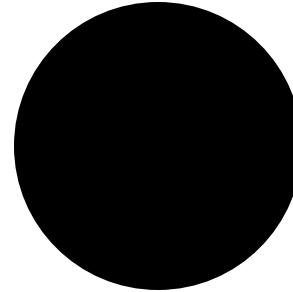
Lab scale
 $d=0.25m$



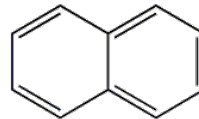
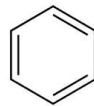
Demonstration scale
 $d=2.5m$



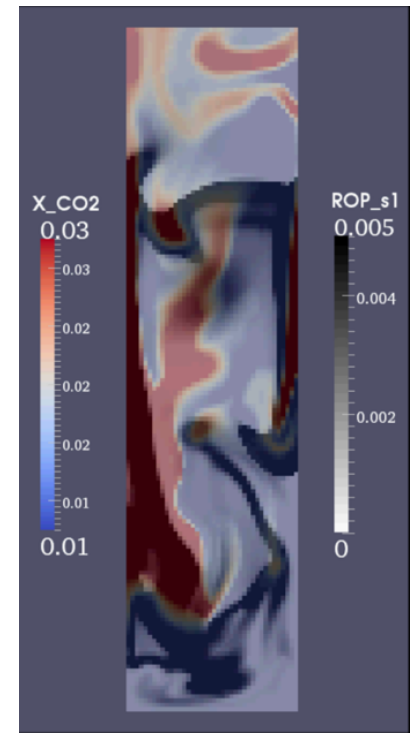
Commercial-scale
 $d=5m$



2. Undesirable tar compounds



3. Complex gas-solid mixing and hydrodynamics



Multiscale-multi physics simulations

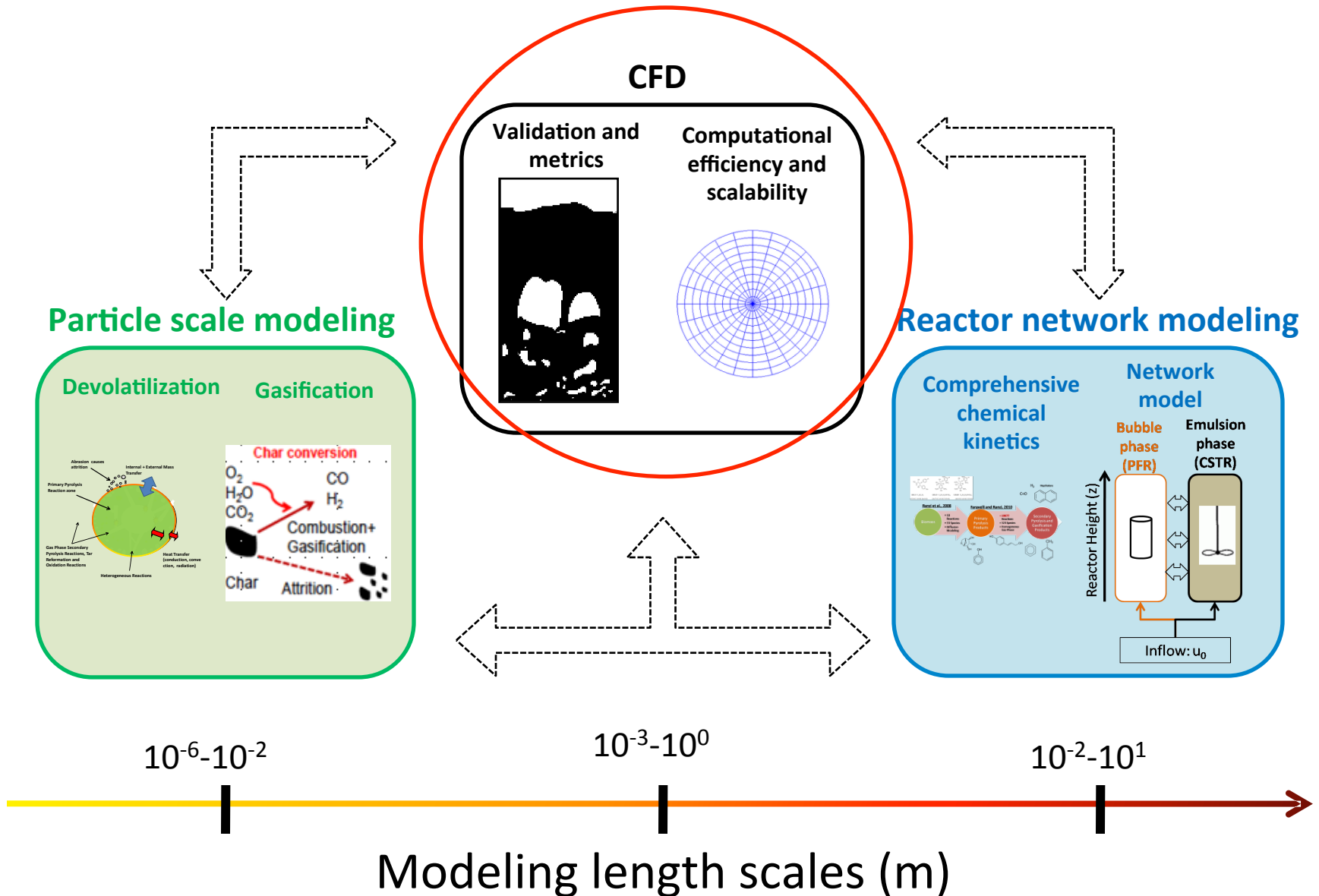
Technical challenges in fluidized bed gasification

1. Expensive scale-up
2. Undesirable tar compounds
3. Complex gas-solid mixing and hydrodynamics

MIT's modeling work

1. Bakshi et al. Efficient computational schemes for cylindrical FB reactors with CFD, *Powder Tech.* 2014. [3]
2. Altantzis et al., Sensitivity of solids circulation to walls, particle, flow characteristics using CFD. , *Powder Tech.*, 2015 [4]
3. Bakshi, et al., Eulerian-Eulerian simulation of dense solid-gas cylindrical fluidized beds; wall boundary condition and its impact on fluidization. *Powder Tech.*, 277 (2015) 47-62 [5]
4. Stark et al., Prediction and validation of syngas and tar species from a reactor network model of fluidized bed biomass gasification, *Energy & Fuels*, 2015 [6]
5. Bates et al, Char combustion, gasification and attrition in bubbling fluidized beds. *Energy & Fuels* 2015 [7]
6. Stark, A., Comprehensive particle and homogeneous chemistry modeling, PhD Thesis 2015 [8]
7. Sridhar, Reactor Network Modeling of biomass gasification with detailed chemistry, Master Thesis 2015.

Towards Multi-scale simulation of biomass gasification



Computational approaches to fluidization

Approach	Gas Phase	Solid Phase	Scale
Discrete Bubble Model	Lagrangian	Eulerian	Industrial (10 m)
Two Fluid Model	Eulerian	Eulerian	Engineering (1 m)
Discrete Element Model	Eulerian (unresolved)	Lagrangian	Laboratory (0.1 m)
Discrete Particle Model	Eulerian (resolved)	Lagrangian	Laboratory (0.1 m)
Molecular Dynamics	Lagrangian	Lagrangian	Mesososcopic (<0.001 m)

Accuracy



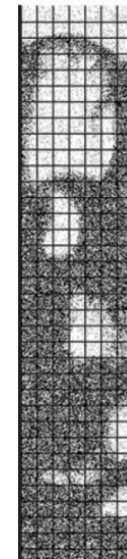
Computational efficiency



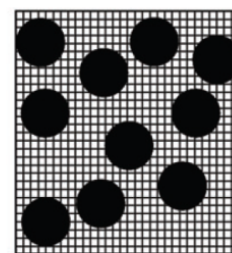
Model 1



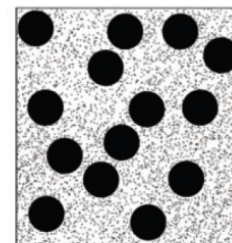
Model 2



Model 3



Model 4

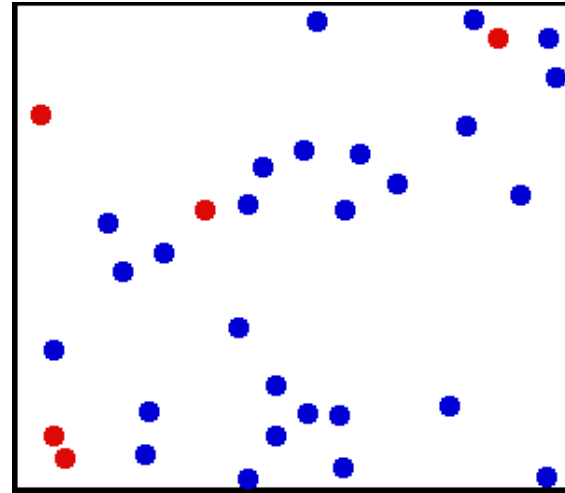


Model 5

Two-Fluid Model (TFM) balances computational efficiency with modeling fidelity making it suitable to industrial scale but challenges remain!

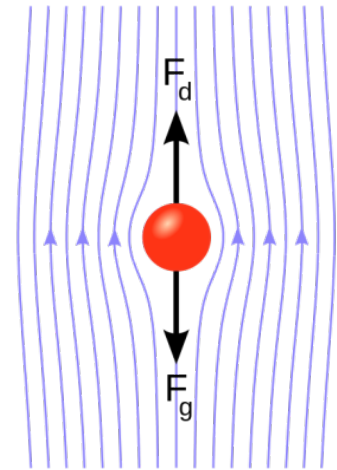
Two Fluid Model

- Particle-Particle interactions
 - Kinetic theory of granular flows
 - Inter-particle drag law
 - Segregation slope coefficient, C_s
 - Friction coefficient, C_f
- Particle-gas interactions
 - Drag laws
- Particle-wall interactions
 - Restitution coefficient, e
 - Specularity coefficient, ϕ

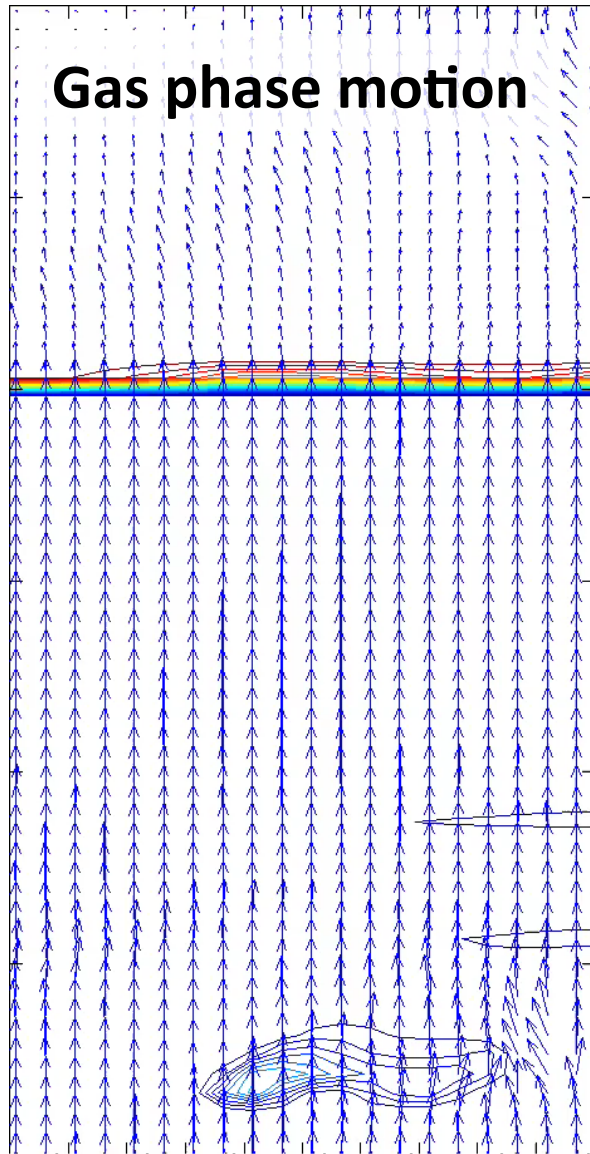


Closure models involve parameters whose influence on hydrodynamics need investigation by means of:

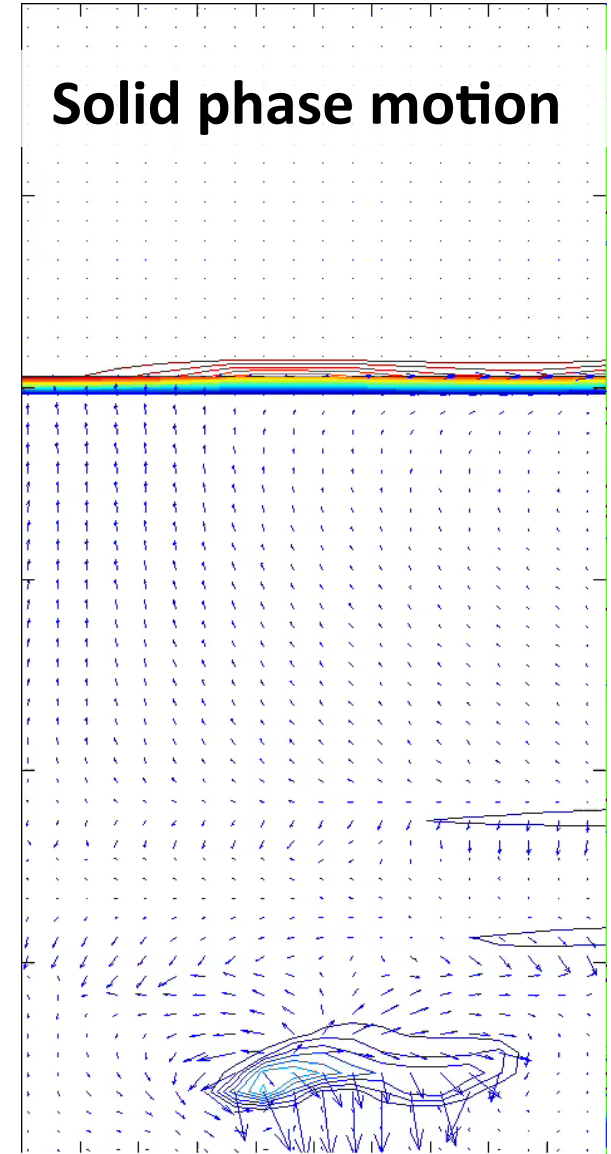
- Detailed experiments
- Validation strategies
- Use of detailed numerical methodologies in smaller scales



Importance of bubble physics during fluidization



- Ascending bubbles drive solids motion
- Bubbles act as pathways for gas flow



Metrics for fluidization hydrodynamics

Original CFD data $f(x,y,z,t)$



Bubble statistics

Dense phase statistics

Velocimetry

Static

Velocimetry

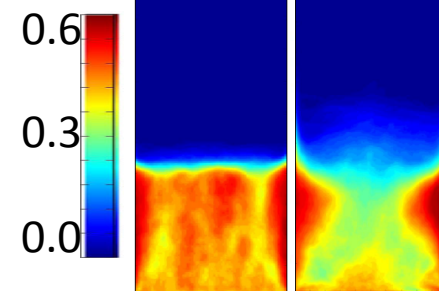
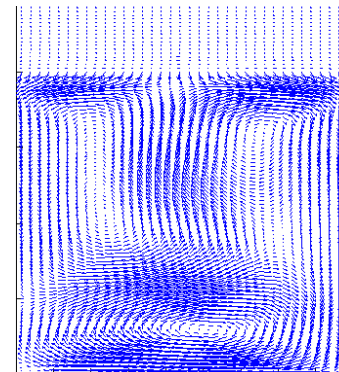
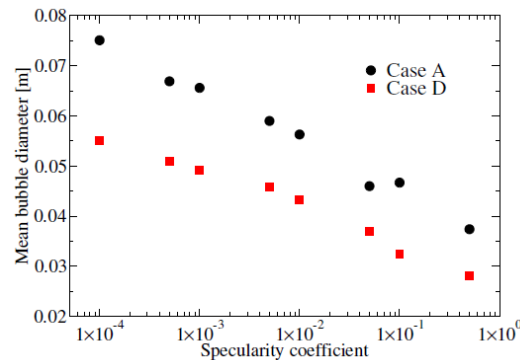
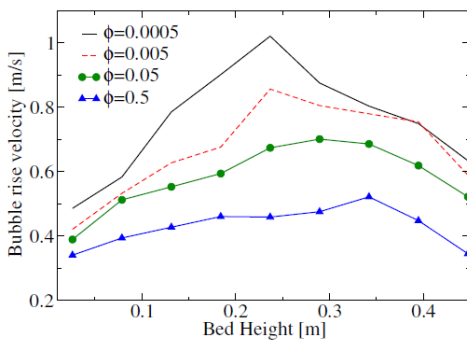
Static

Velocity vs Height

Size vs height

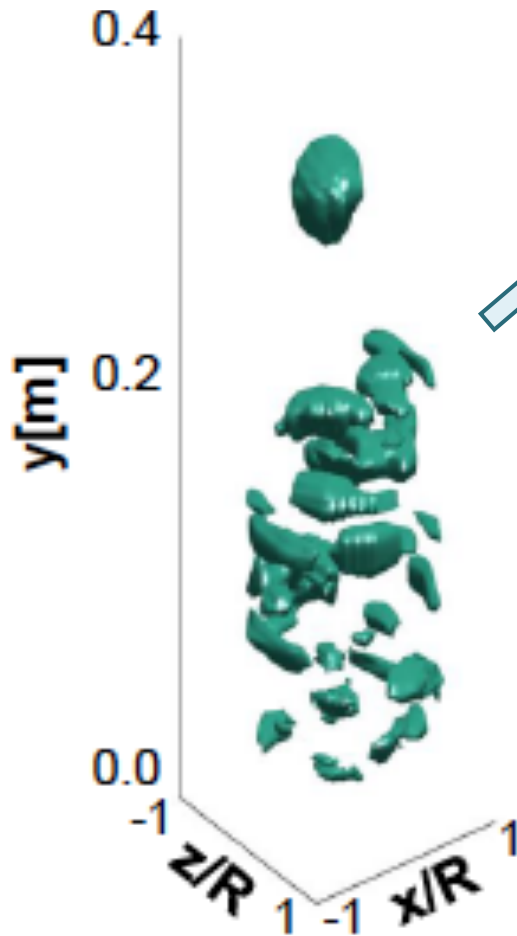
Circulation flux

Time mean solids holdup

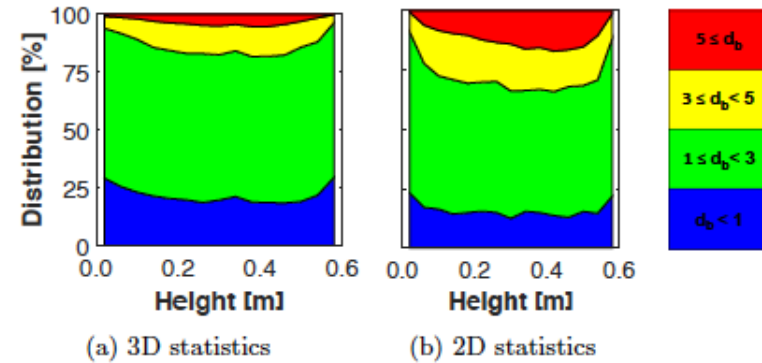


3D bubble statistics tool

Bakshi at.al,



Statistical analysis of
bubble size and
velocity distributions

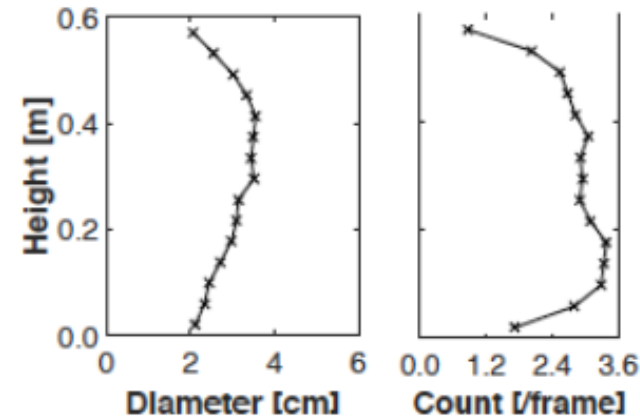


Bubble geometric characteristics

- Surface area
- Volume
- Cord length (axial/radial)
- Aspect ratios

3D bubble analysis for:

- Accurate detection of the number of bubbles in the bed (only a fraction is captured with 2D analysis)
- Azimuthal motion of bubbles



Dense phase mixing metric

- Circulation fluxes & circulation times are sensitive to the parameters in sub-models
- Useful quantities for rigorous quantitative validation with novel experimental measurements employing particle velocimetry
- Strongly coupled with the bubbling behavior in the bed

Time mean **solid's circulation flux up** $J_c^+(y)$ based on the upflow area $A^+(y)$ i.e.

$$J_c^+(y) = \left\langle \frac{1}{A^+(y,t)} \int \int \rho_m \cdot \varepsilon_m \cdot v_m^+ dA^+ \right\rangle \quad v_m^+ = \begin{cases} v_m & \text{if } v_m > 0 \\ 0 & \text{otherwise} \end{cases}$$

$$v_s^+(y) = \left\langle \frac{\int \int \varepsilon_m \cdot v_m^+ dA^+}{\int \int \varepsilon_m dA^+} \right\rangle \quad dA^+ = \begin{cases} dA & \text{if } v_m > 0 \\ 0 & \text{otherwise} \end{cases}$$

$$t_c^+(y_1, y_2) = \int_{y_1}^{y_2} \frac{\Delta y}{v_s^+(y)} dy$$



The total **solid's circulation time** $t_c(y_1, y_2) = t_c^+(y_1, y_2) + t_c^-(y_1, y_2)$ is representative of the mixing time scale

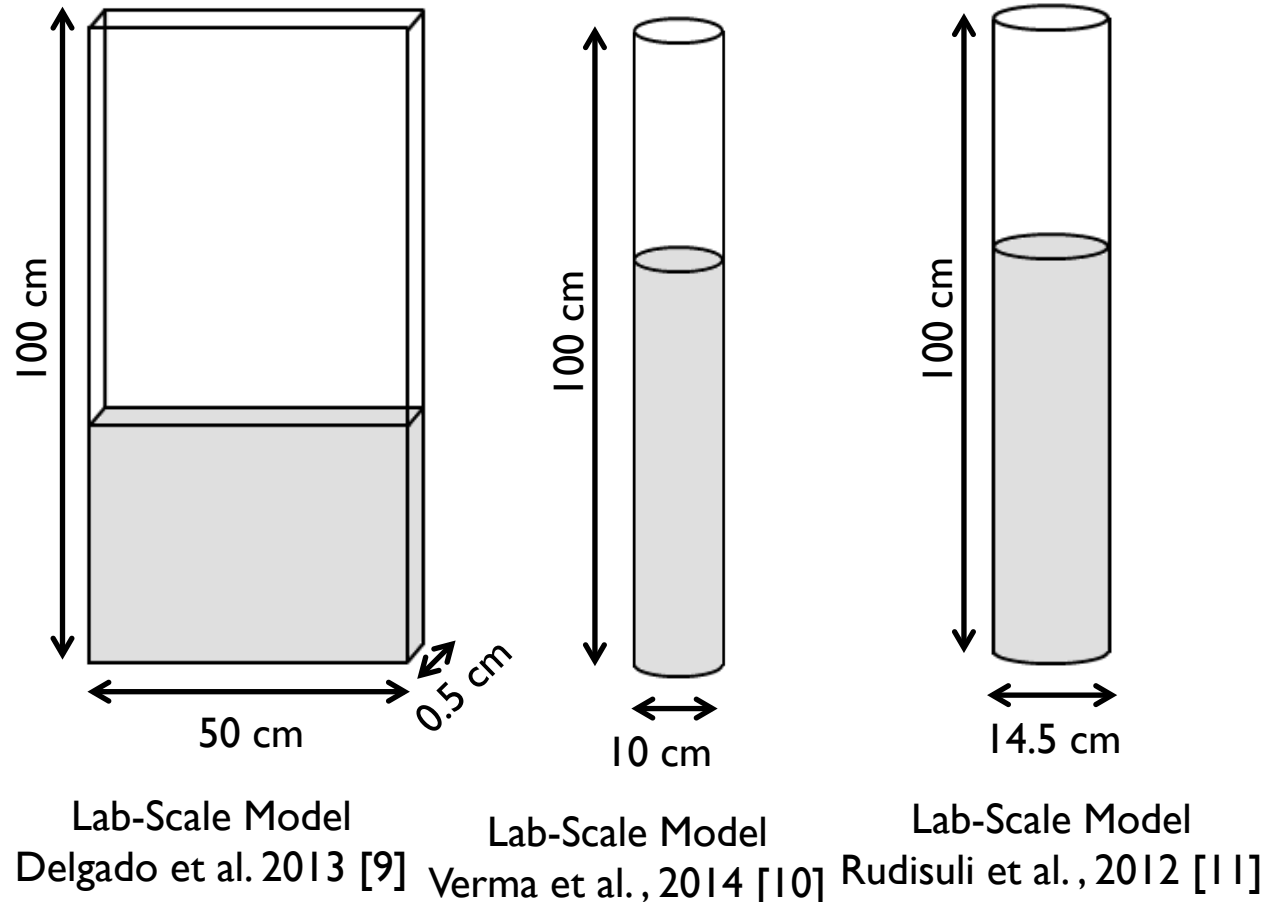
Parameter estimation and validation strategy

Example: specularity coefficient

- Lack of experimental data on $\phi_w \Rightarrow \phi_w$ is a fitting parameter

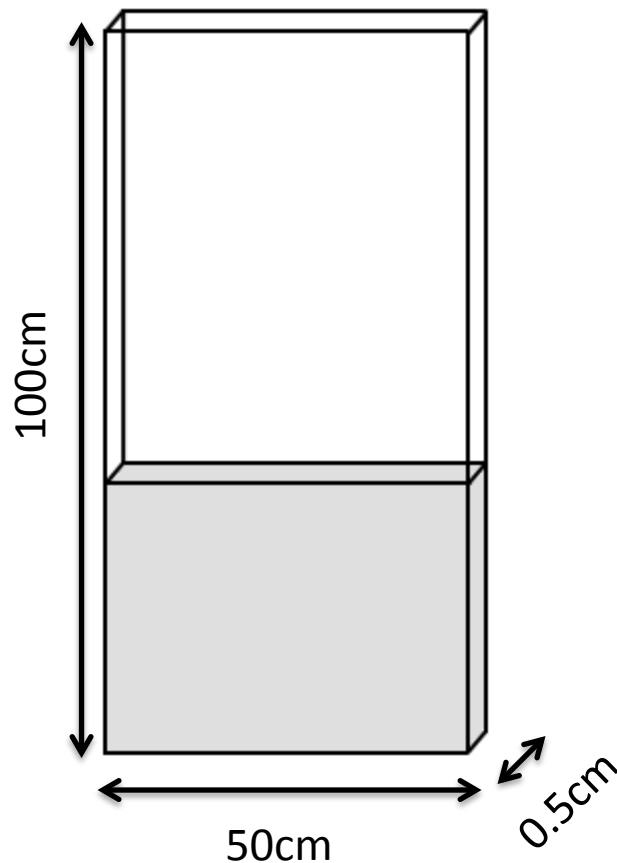
ϕ_w tuned to 2D simulations is not appropriate for 3D simulations

- Thin rectangular beds extensively used in **experimental studies** employing non-intrusive measurements techniques
- Cylindrical beds **more realistic** geometries for scale-up and different hydrodynamics compared to pseudo-2D beds
- Variation of specularity coefficient to evaluate impact on simulation of pilot-scale model



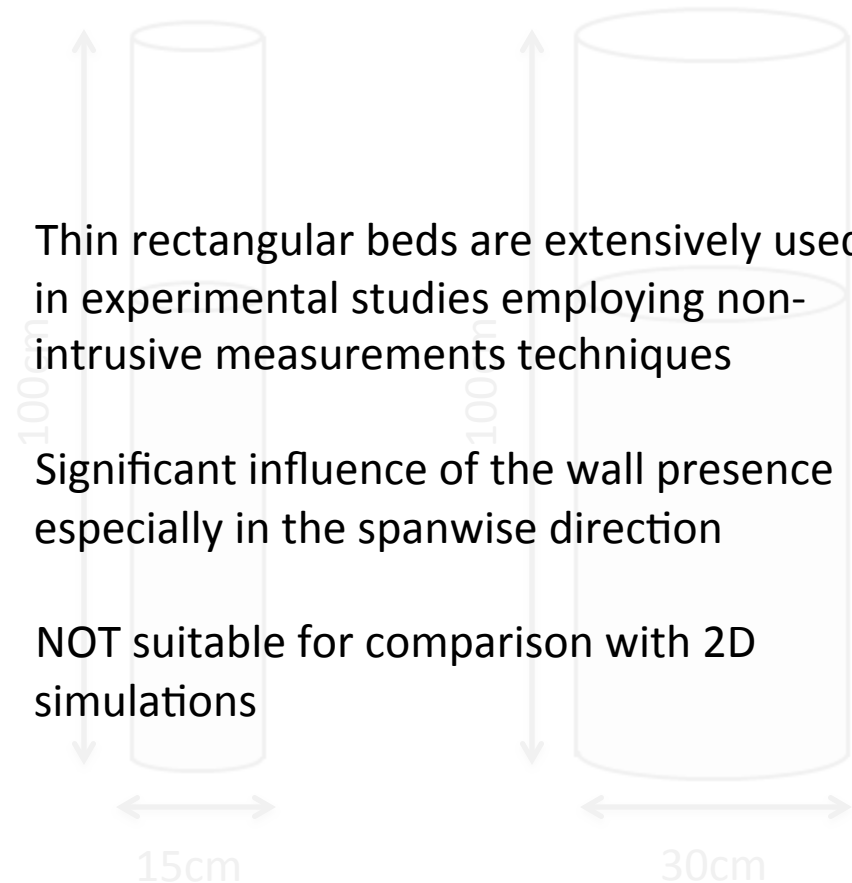
Parametric analyses and validation

- Parametric analyses with respect to the specularity coefficient
- Validation based on experimental studies for sand-like particles in different bed geometries



Delgado et al. 2013 [9]
(Digital Image Analysis
for solids motion)

- Thin rectangular beds are extensively used in experimental studies employing non-intrusive measurements techniques
- Significant influence of the wall presence especially in the spanwise direction
- NOT suitable for comparison with 2D simulations

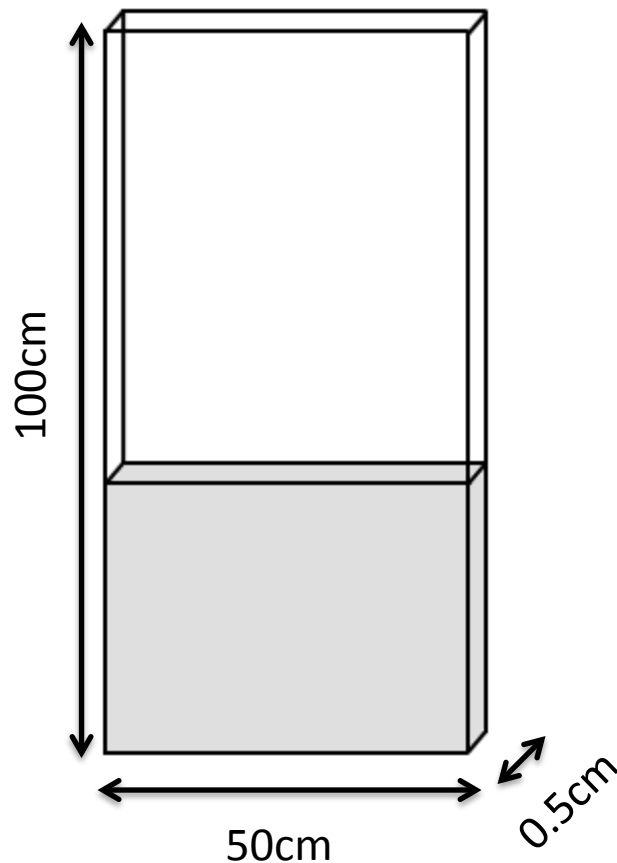


Rudisuli et al., 2012
(Optical probe measurements
for bubble dynamics)

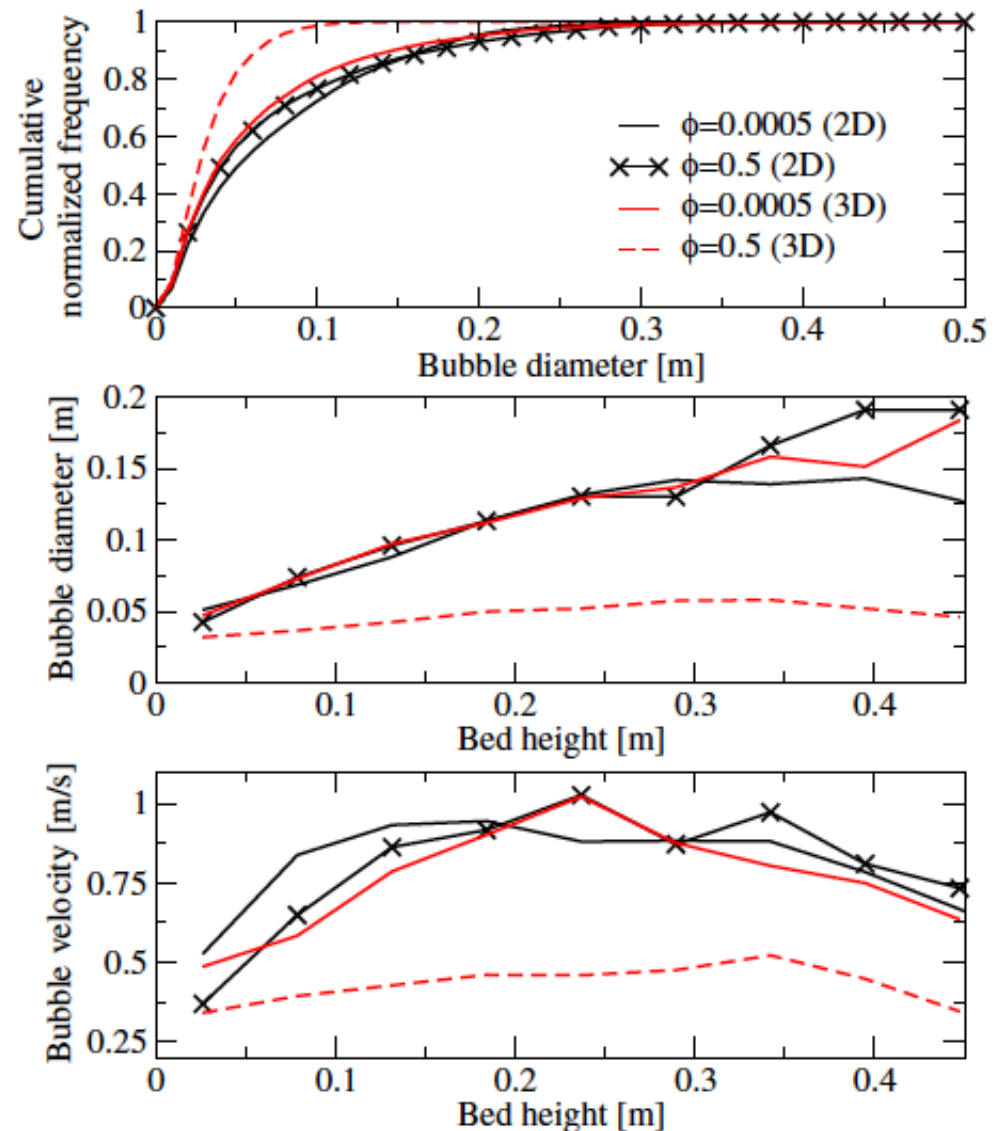
Pilot scale reactor

Parametric analyses and validation

- Parametric analyses with respect to the specularity coefficient
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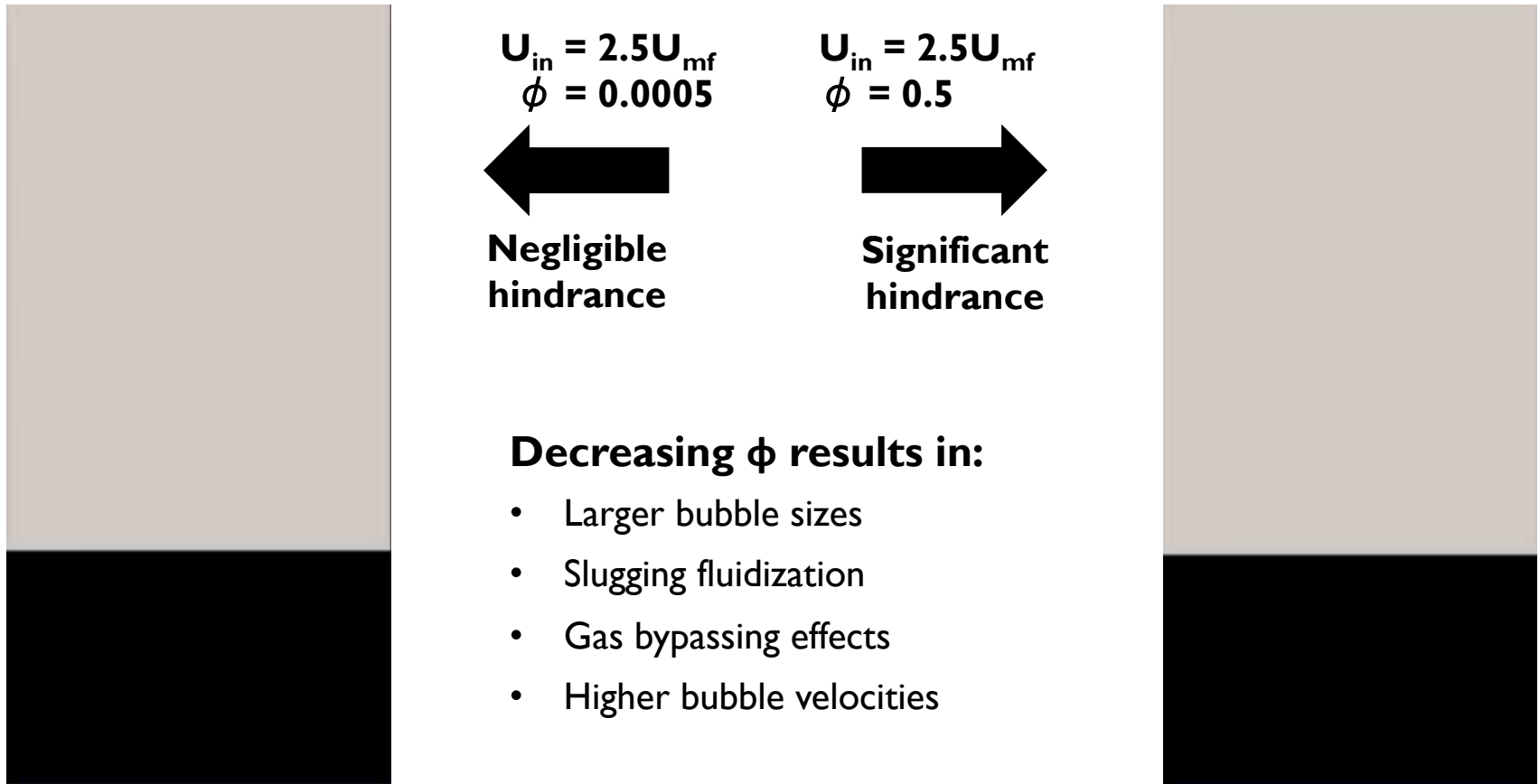
Delgado et al. 2013
(Digital Image Analysis
for solids motion)



Thin rectangular bed

Simulation Results

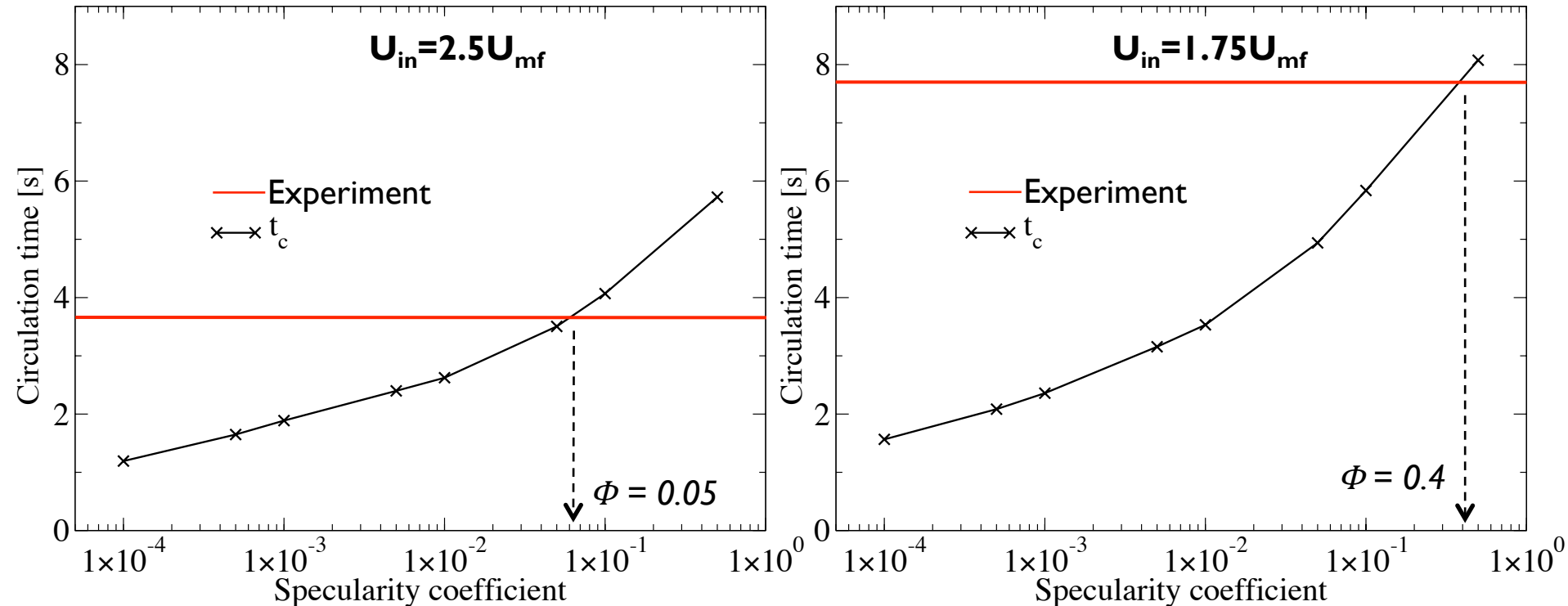
Bubble hydrodynamics and solids motion significantly influenced by wall boundary condition



Thin rectangular bed

Choosing Φ

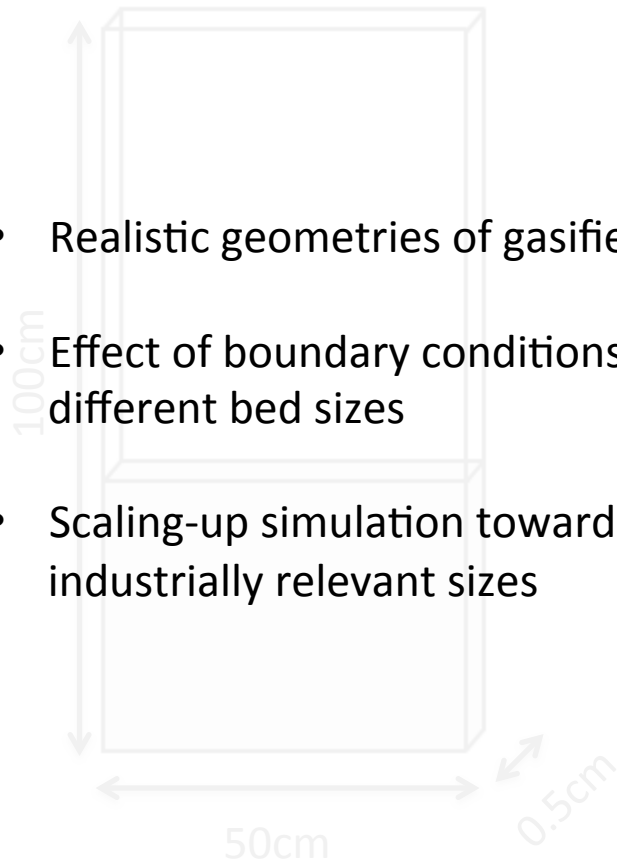
- Circulation time $\uparrow$ when
 - $U_{in} \downarrow$ - closer to U_{mf} and less bubbling
 - $\phi \uparrow$ - wall resistance increases $\Rightarrow$ less solid motion close to walls and smaller bubbles
- **Appropriate $\phi \downarrow$ as $U_{in} \uparrow$.** For the range, $1.5U_{mf} - 2.5U_{mf}$, $\Phi \in [0.05, 0.5]$



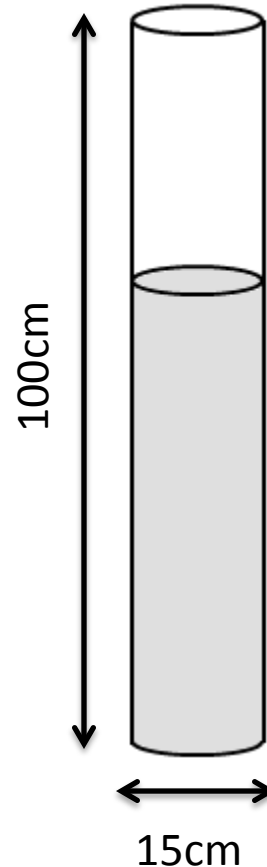
Parametric analyses and validation

- Parametric analyses with respect to ϕ and the drag model
- Validation based on experimental studies for sand-like particles in different bed geometries

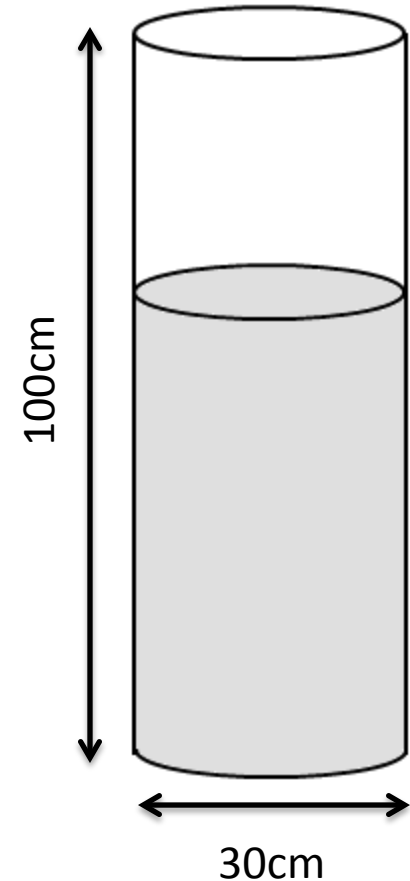
- Realistic geometries of gasifiers
- Effect of boundary conditions for different bed sizes
- Scaling-up simulation towards industrially relevant sizes



Delgado et al. 2013
(Digital Image Analysis
for solids motion)



Rudisuli et al. , 2012 [11]
(Optical probe measurements
for bubble dynamics)

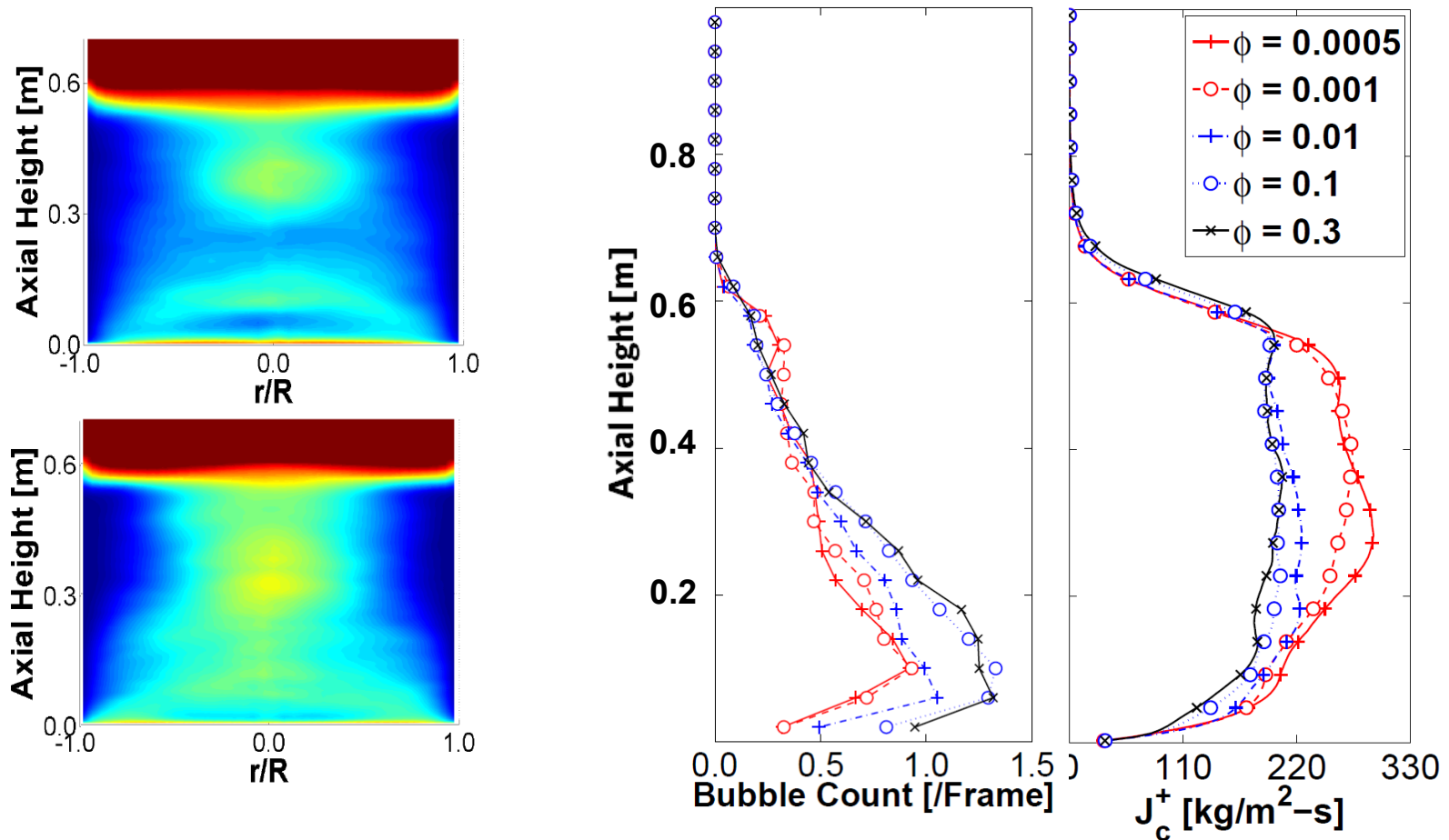


Pilot scale reactor

Influence of specularity coefficient in a 3D cylindrical bed

Mechanism

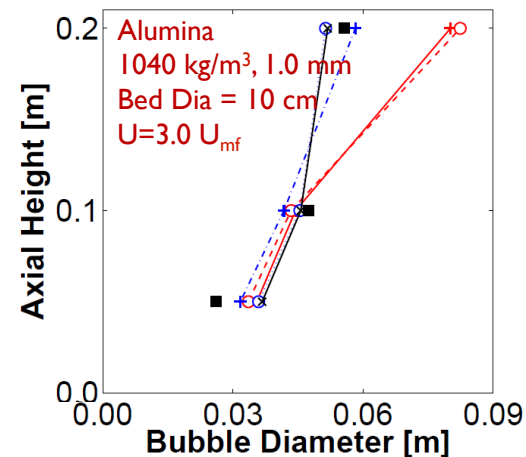
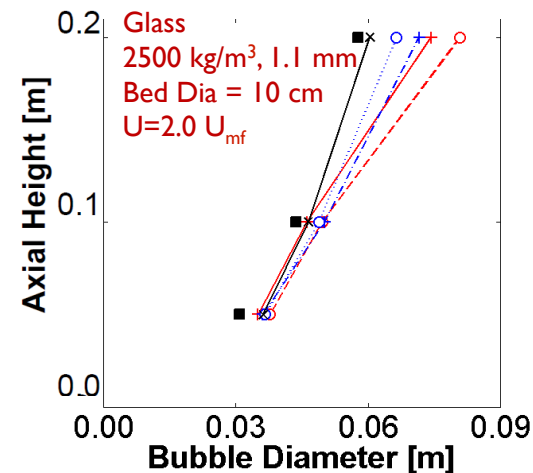
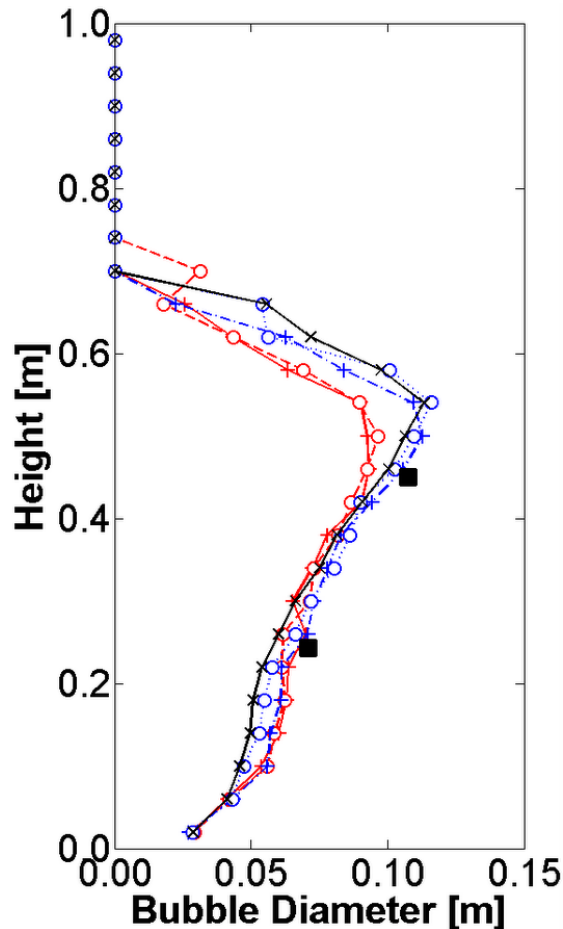
$\phi \Rightarrow v_s^{+/-} \Rightarrow$ solids distribution (circulation flux / time) bubble dynamics (Bubble dia/count)



Validation

Suitable ϕ ?

- Range – $1.25-6.80 U_{mf}$, $860-2500 \text{ kg/m}^3$, $0.289-1.1 \text{ mm}$
- Bubble diameter comparisons show higher values of ϕ (0.01-0.3) more suitable for dense flows
- Low sensitivity of metrics (solids / bubbles) for suitable ϕ
- Variable ϕ model (Li&Benyahia [12]) matches the results of the suitable ϕ



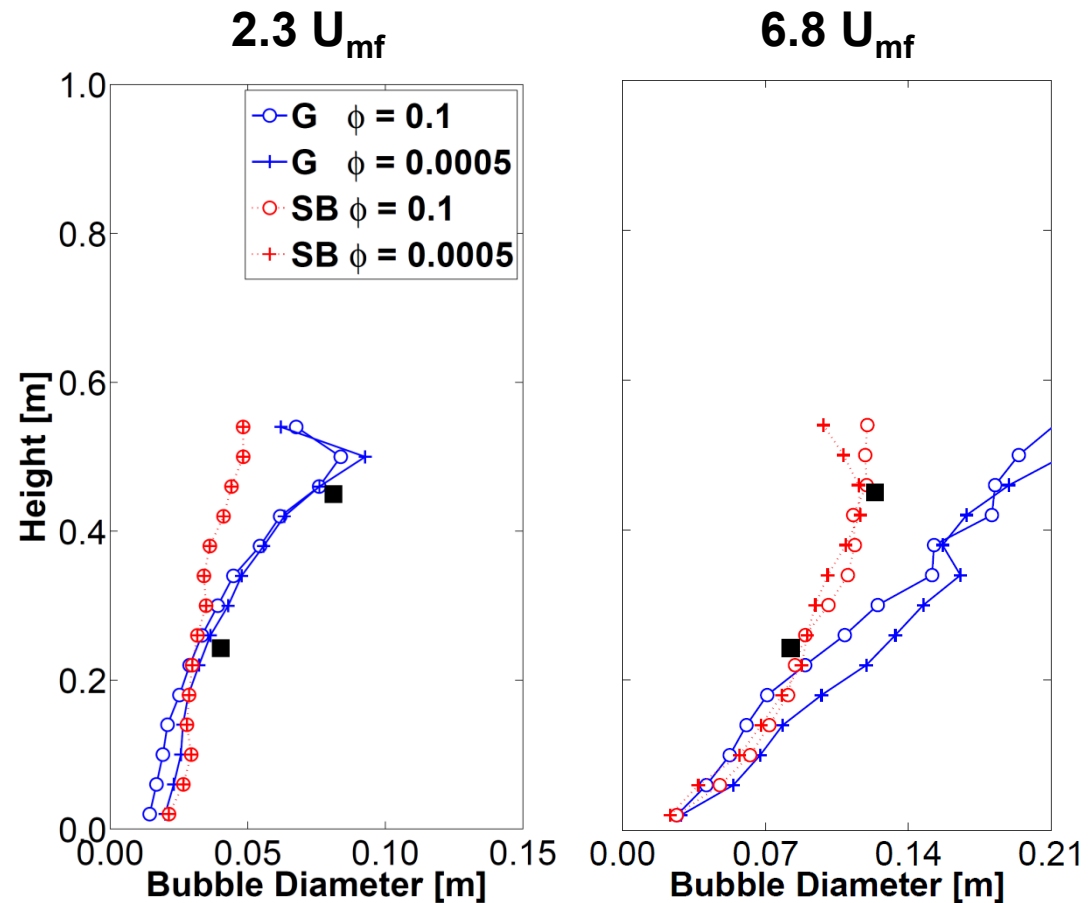
Influence of drag model

Effect on Pilot-Scale Bed

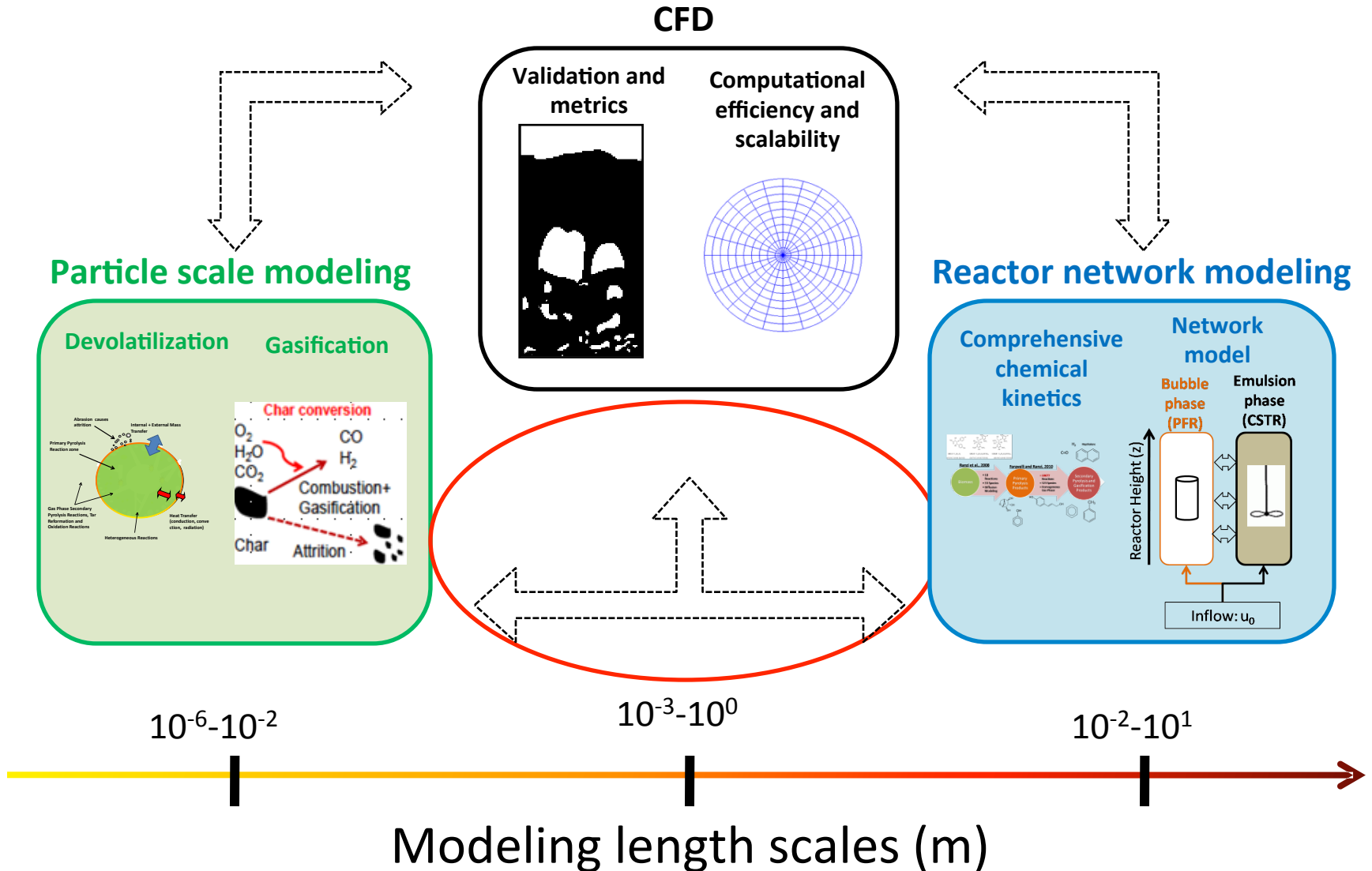
- Gidaspow model = pressure drop data from packed + homogeneous fluidization experiments
- Syamlal-O'Brien model = terminal velocity correlation of particles from liquid-solid beds

Takeaways -

1. Drag model has a strong impact on fluidization
2. Gidaspow model more suited for low velocities (2-4 U_{mf})



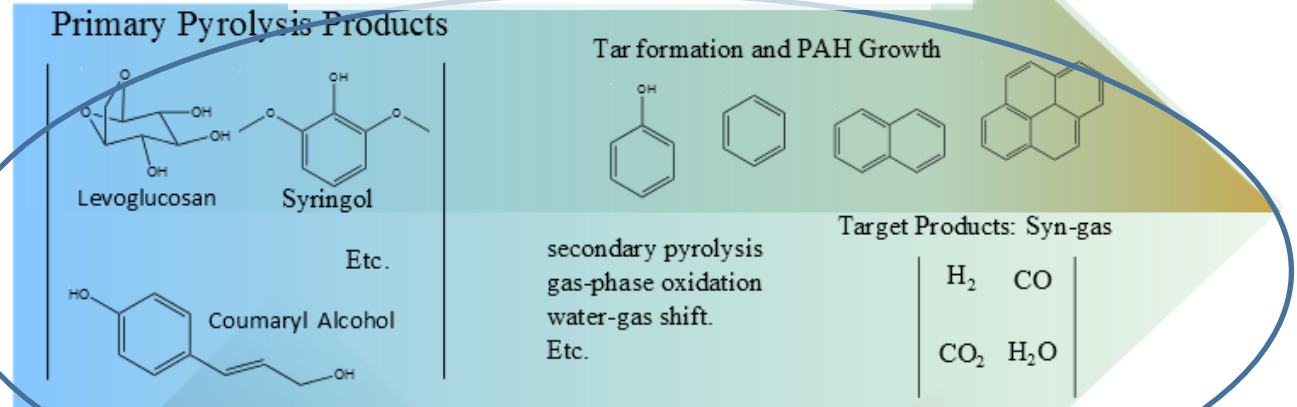
Towards Multi-scale simulation of biomass gasification



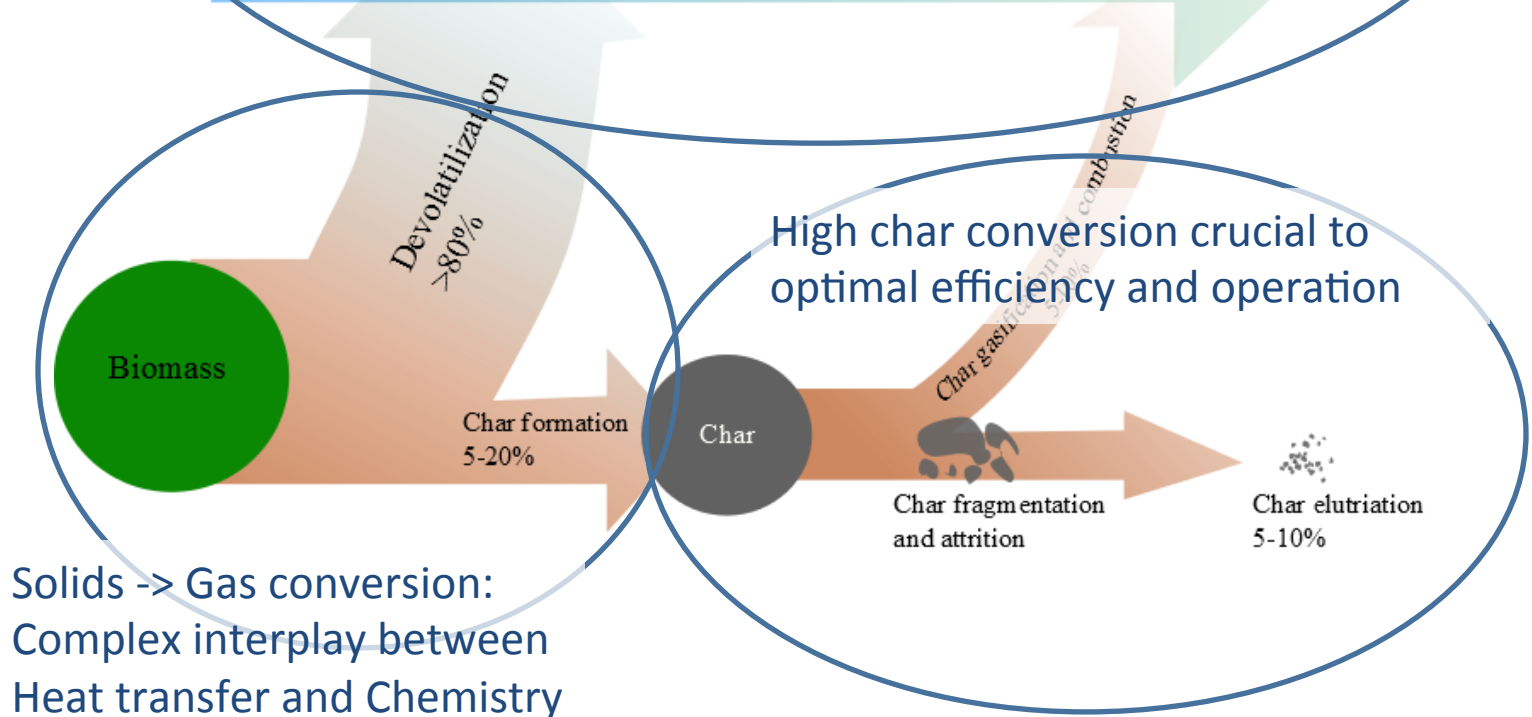
Thermochemical Conversion of Biomass in FBBG

Gas-Phase Reactions:
Multiple species and pathways

Gas-Phase
Conversion
Pathway

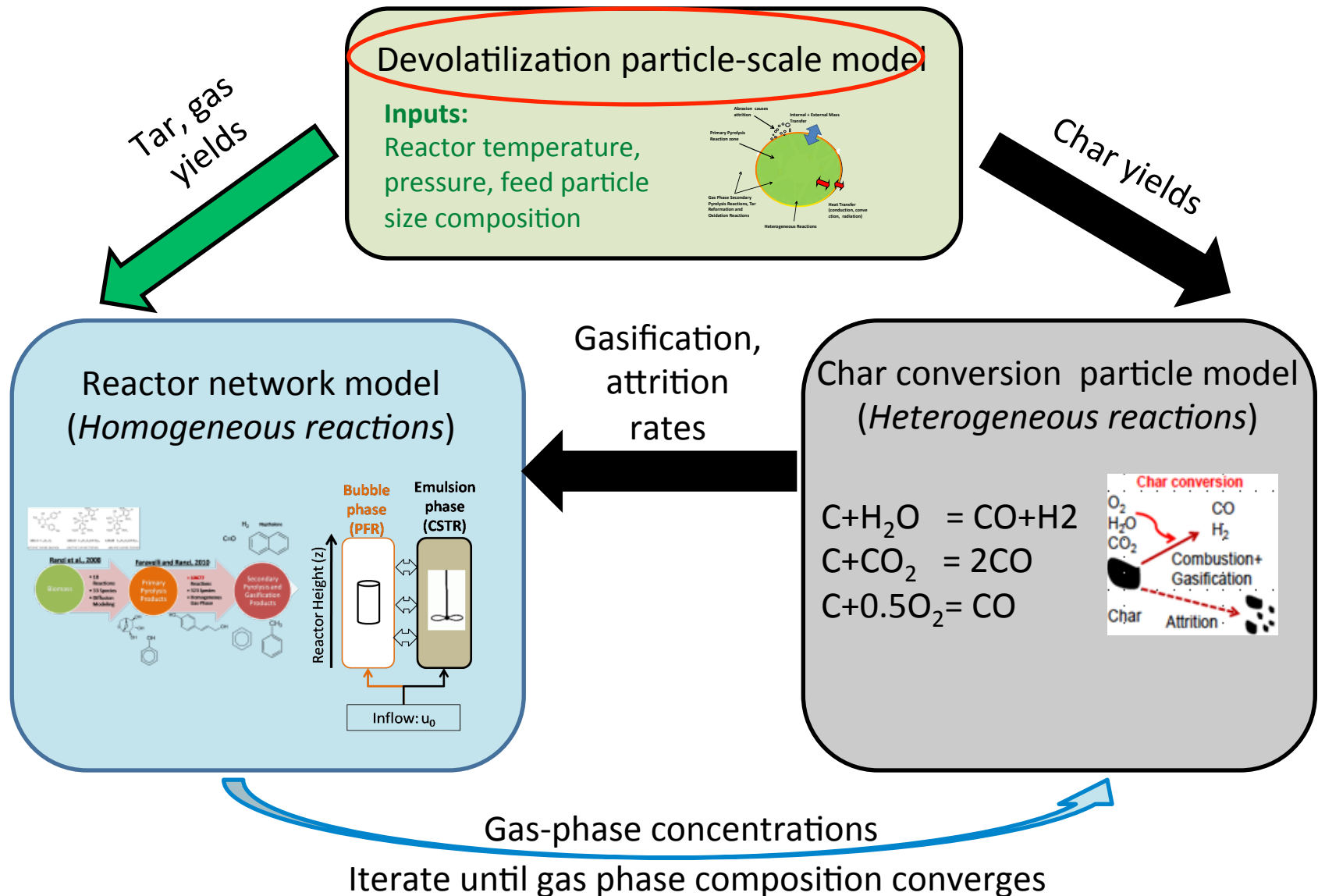


Solids
Conversion
Pathway



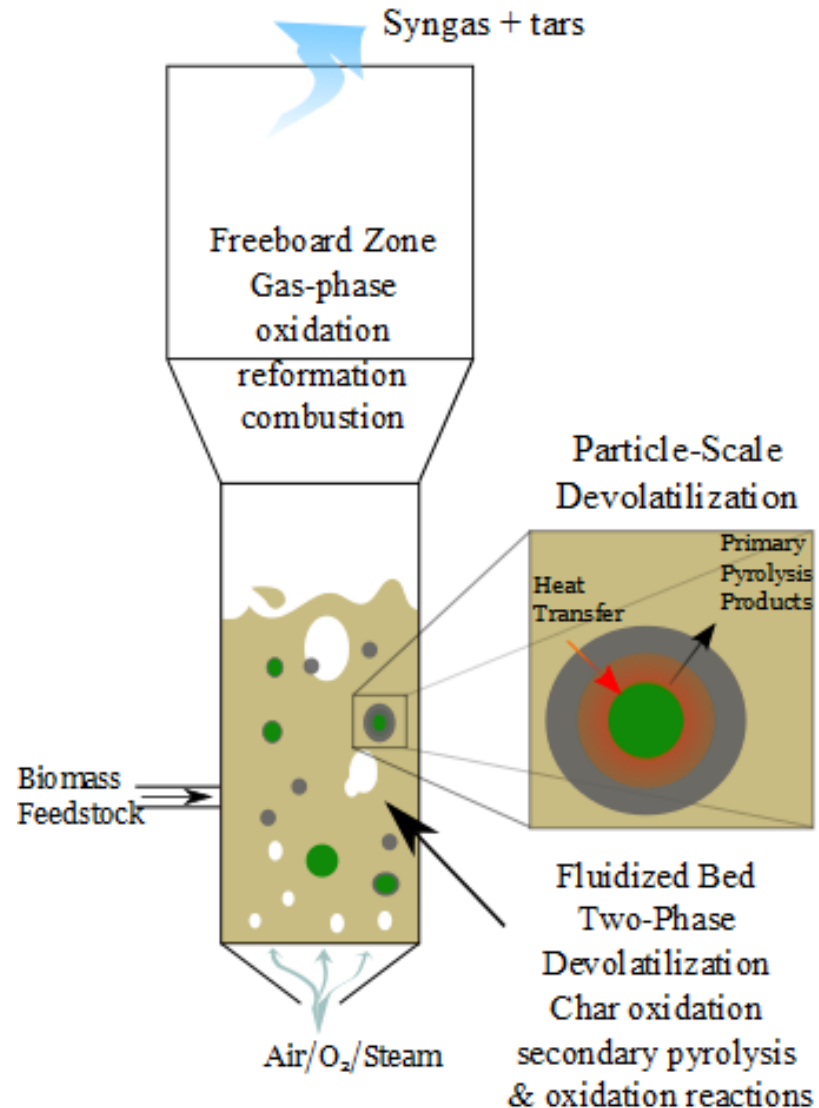
Solids -> Gas conversion:
Complex interplay between
Heat transfer and Chemistry

Approach: Integrated particle/reactor network models to predict gasifier outputs



Transport limitations during particle-Scale devolatilization

- ▶ Particle-phenomena directly influence overall conversion
- ▶ Interplay between
 - ▶ External convective heat transfer from the bed to the particle
 - ▶ Internal conductive heat transfer
 - ▶ Primary pyrolysis reaction kinetics

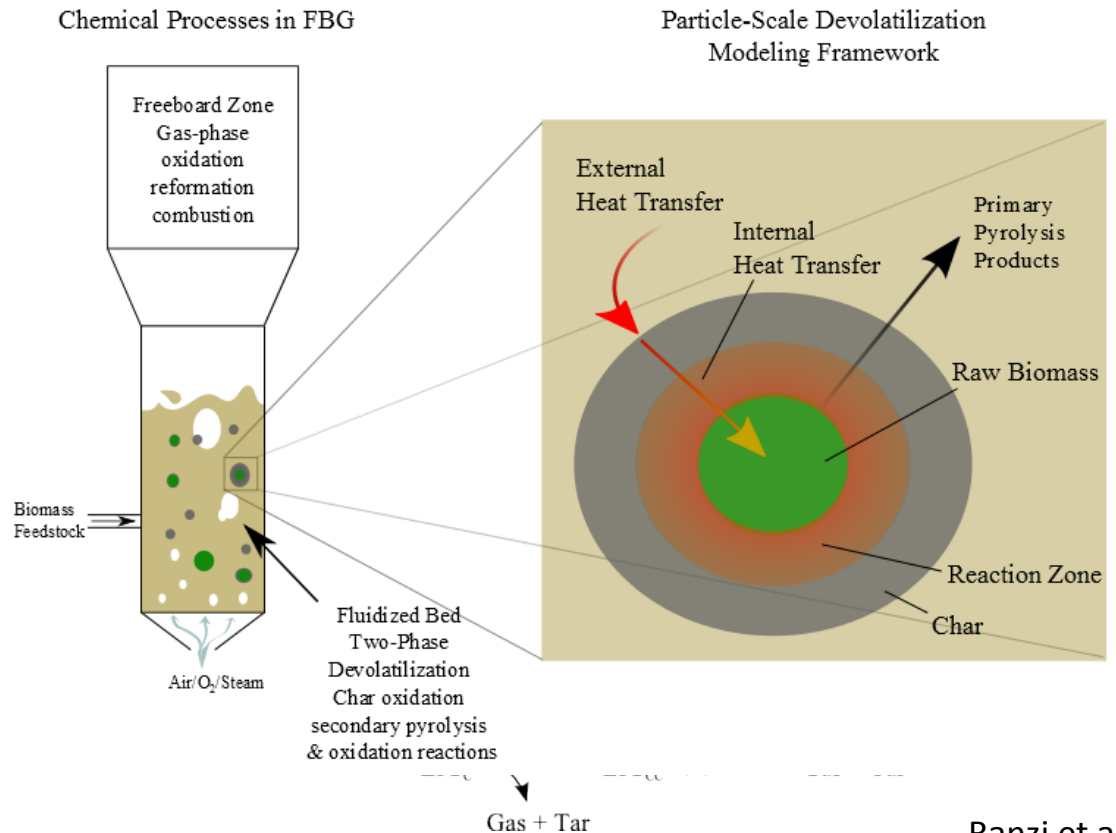


Devolatilization Model Development

1-D particle model

- Base of model is integration of heat transfer and chemical conversion:
 - 1-D heat equation coupled with reactions
 - Mechanism of Ranzi et al. [1]
- Boundary Conditions:
 - *Convective and radiative heat transfer at surface from particle trajectory history*
 - *Can come from CFD!*
- System of equations are integrated with respect to time.
 - Requires a stiff ODE integrator.
 - Simulation cost: 100 cpu-seconds per second.

Devolatilization Mechanism

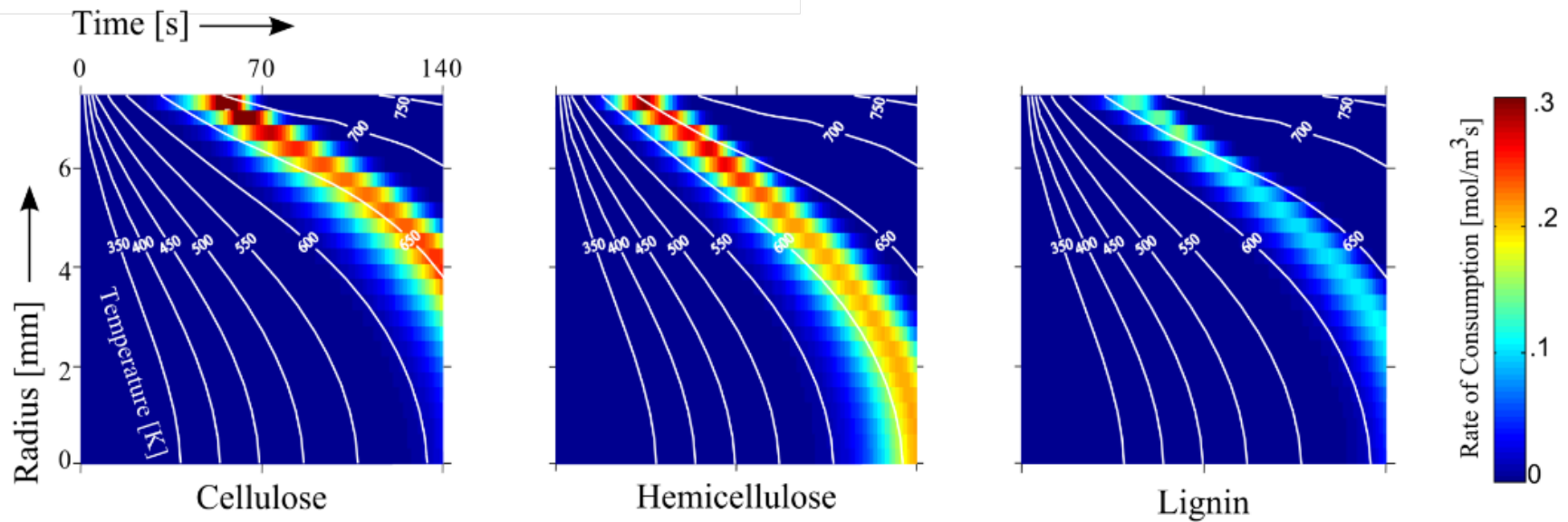


Ranzi et al. [1]

Single Particle Model Predictions

Resolves internal gradients and reaction dynamics

Cellulose, Hemicellulose and Lignin devolatilize sequentially, yielding a triple pyrolysis wave

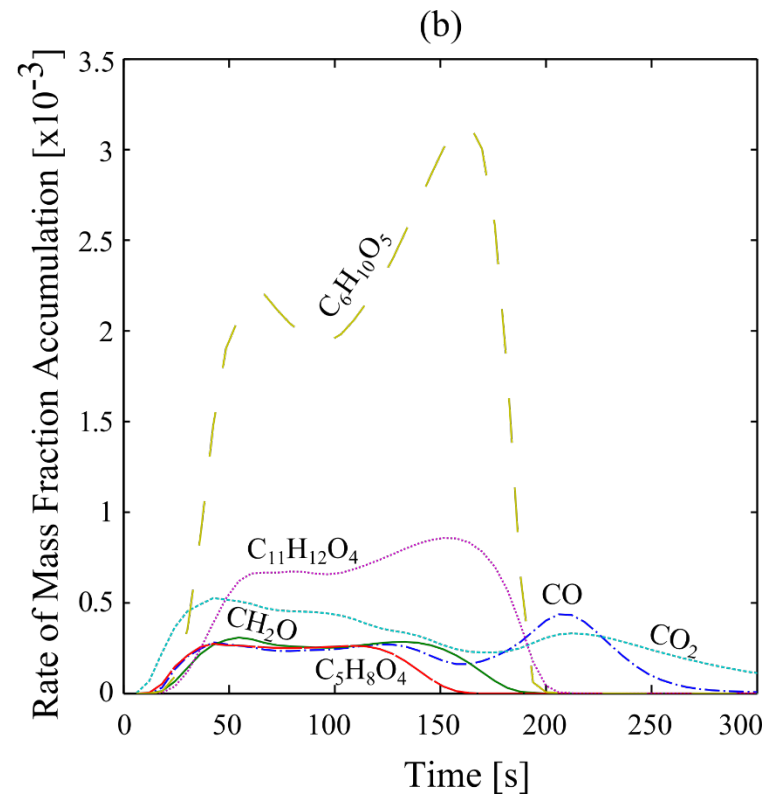
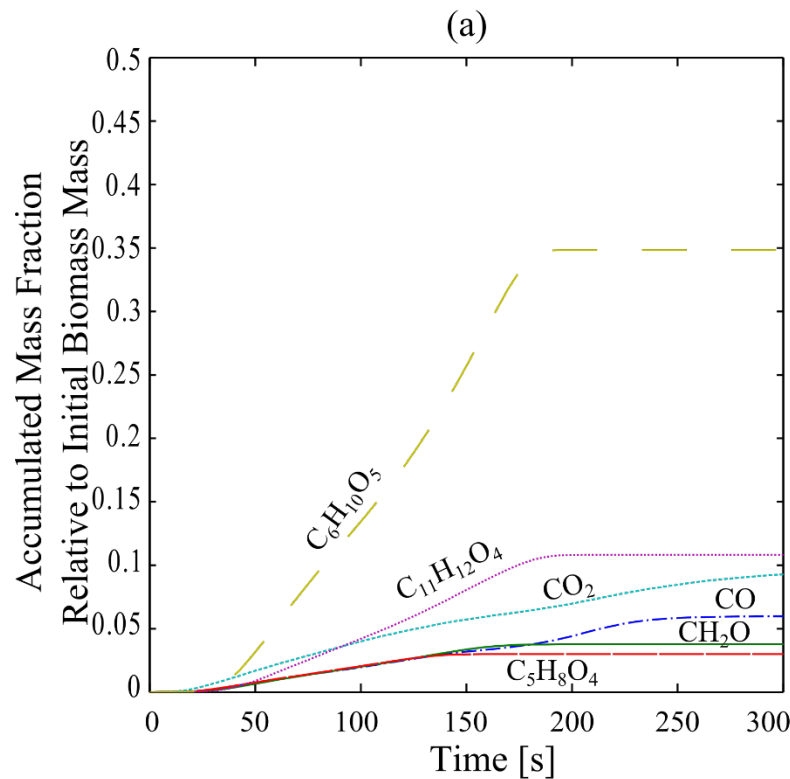


Single Particle Model Predictions

Rate of production of tar precursors are of particular interest. Physical parameters have a strong effect.

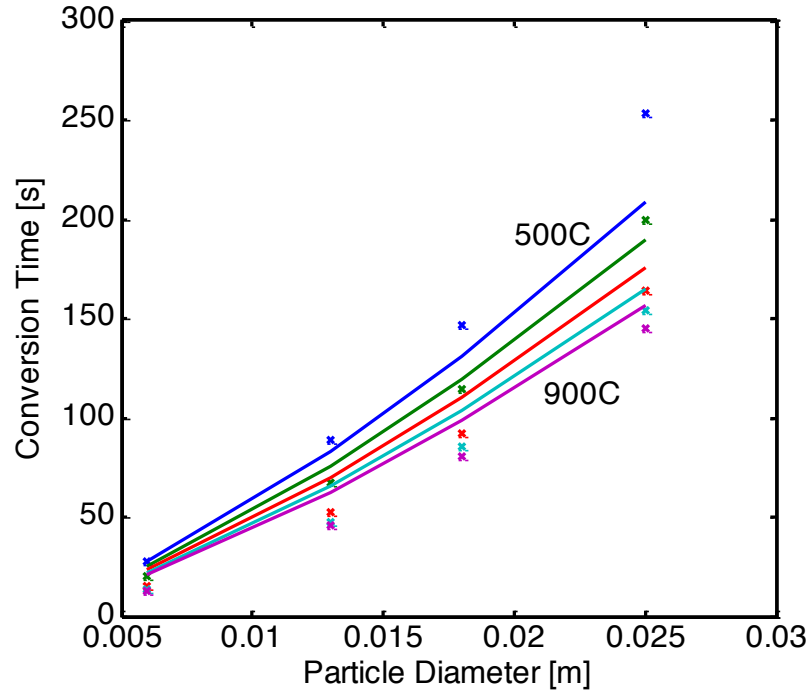
Prediction of Devolatilization Species

20 gaseous species and char

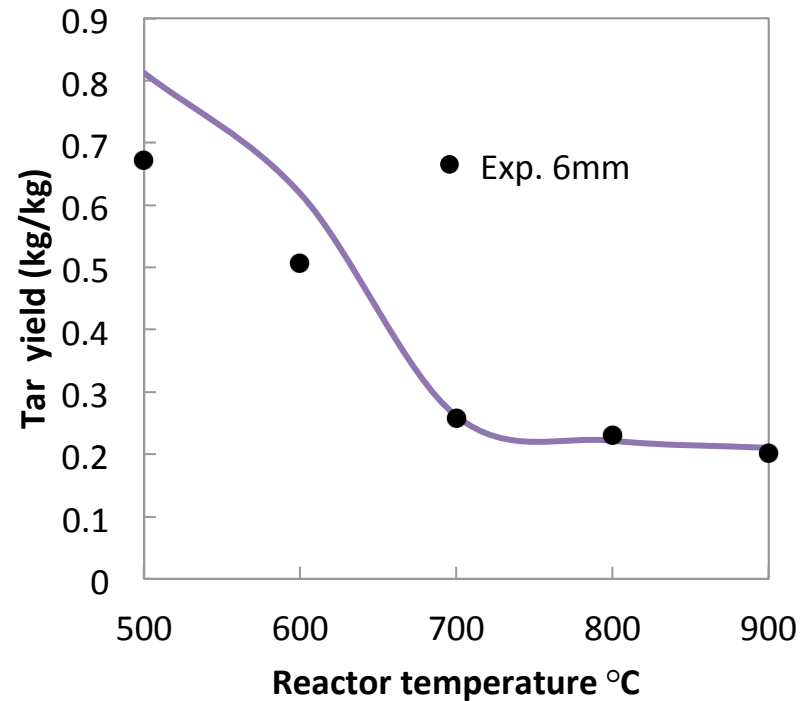


Particle scale devolatilization model validation

Particle devolatilization time versus particle size



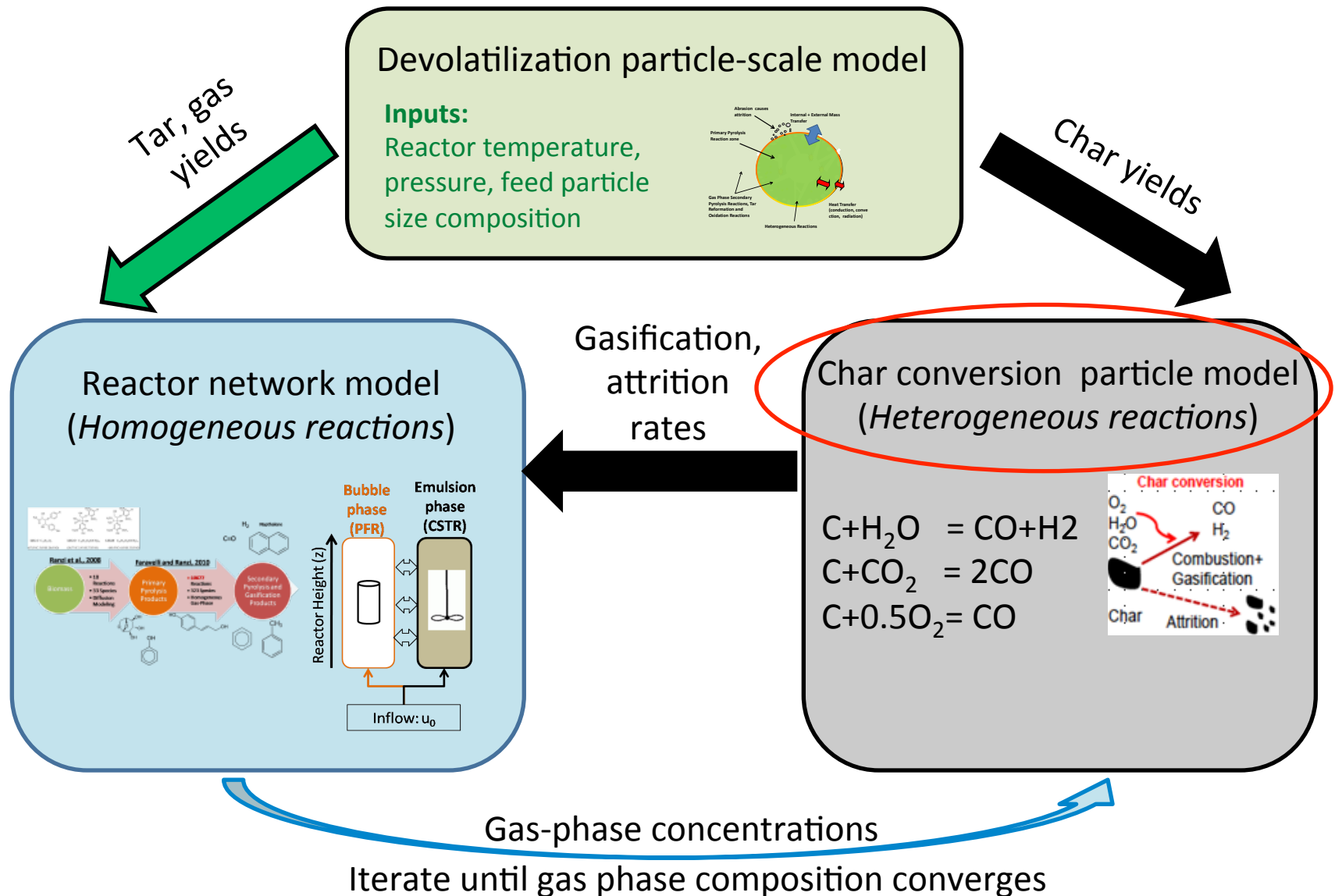
“Tar+water” yields versus reactor temperature



Lines: Best-fit by Gaston et al. 2011 [13]

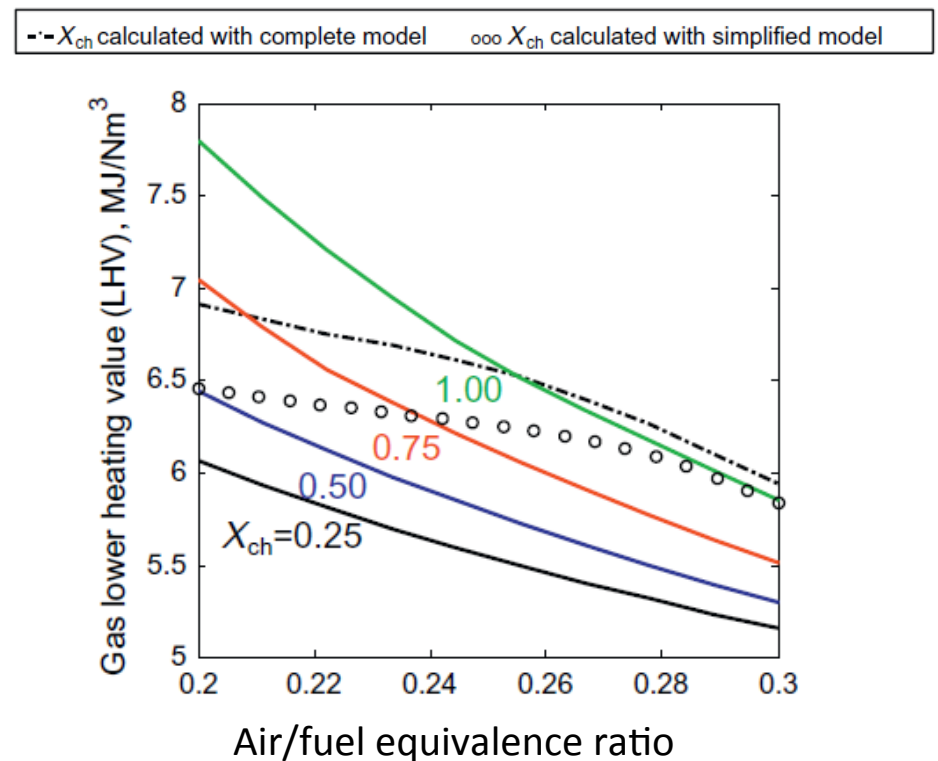
Points: Model predictions

Approach: Integrated particle/reactor network models to predict gasifier outputs



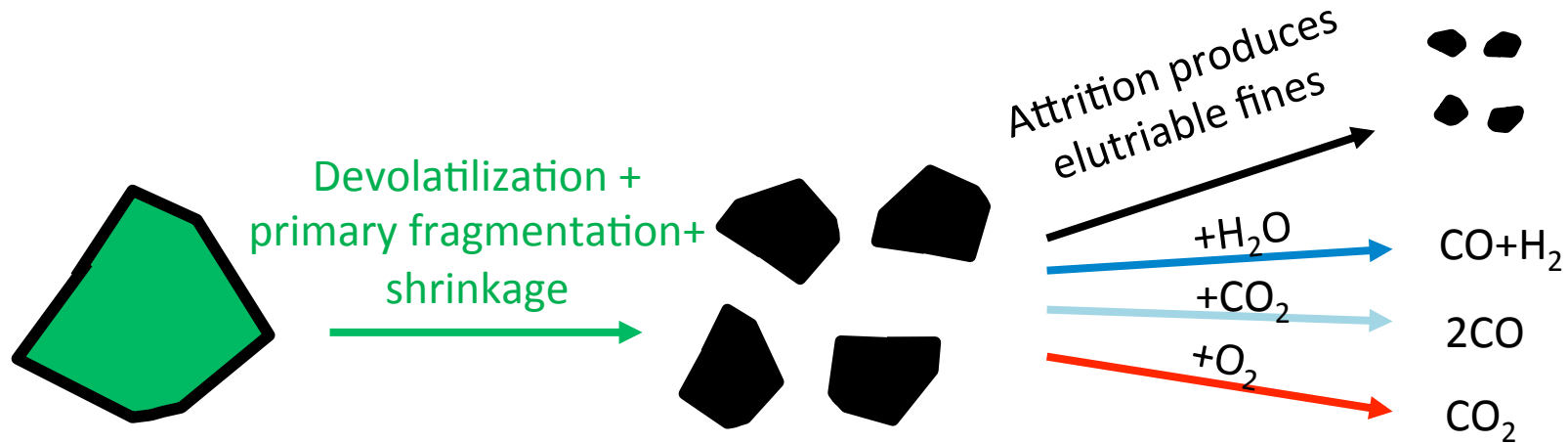
Role of char conversion during FBG

- Gomez-Barea & Leckner 2013 [14]:
- ***“The conversion of char is the most decisive factor in FBG, because the main loss of efficiency is due to unconverted carbon in the ashes.”***
- *“...results show that value assigned for char conversion has a major effect on the temperature, gas heating value, and therefore on other parameters like gas composition and cold gas efficiency”*
- LHV ranges 5.4-7.75 MJ/Nm³ depending on assigned char conversion.
- Char conversion needs to be predicted accurately to reduce uncertainty in major output variables



Calculations for air-blown pilot scale wood pellet FBG by Gomez-Barea & Leckner 2013 [14]:

Char Particle Conversion Model



$$d_{ch,0} = d_{f,0}/(\phi n_1)^{1/3}$$

$n_1 = \text{Fragmentation factor} \sim 4.5$

$\phi = \text{Shrinkage factor} \sim 1.7$

$$dm_{ch}/dt = -(r_{gasif} + r_{attr} + r_{comb})m_{ch}$$

$$d\rho_{ch}/dt = -r_{gasif}\rho_{ch}$$

Assumption	Justification
Fines produced by attrition are assumed to be elutriated as soon as they are produced	Elutriation time scale is fast compared to attrition time scale
Intraparticle diffusion limitations negligible during gasification, dominant during combustion	Thiele modulus $\ll 1$ for gasification Thiele modulus $\gg 1$ during combustion
Isothermal particle	$Bi < 1$

Modified attrition kinetics rate expression

- Attrition acts to reduce the diameter of the char particle
- Attrition rate expression from Scala et al. 2006

$$r_{attrition} \left[\frac{1}{s} \right] = \frac{K_{att}(u_0 - u_{mf})}{d_{char}} F_{att}$$

- Attrition rate modified with a structural attrition profile F_{att} that depends on char density/hardness:

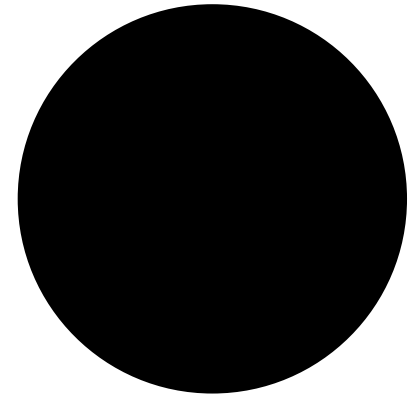
$$F_{att}(X_\rho) = (1 - X_\rho)^{-q} = (\rho_{ch}/\rho_{ch,0})^q$$

- q is fitted for each feedstock

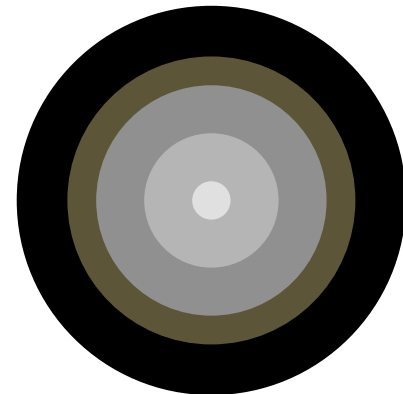
$$10^{-7} < K_{att} < 10^{-8}$$

depending on feedstock/hardness

Existing models do not account for the reduction in density/hardness during conversion to affect the attrition rate

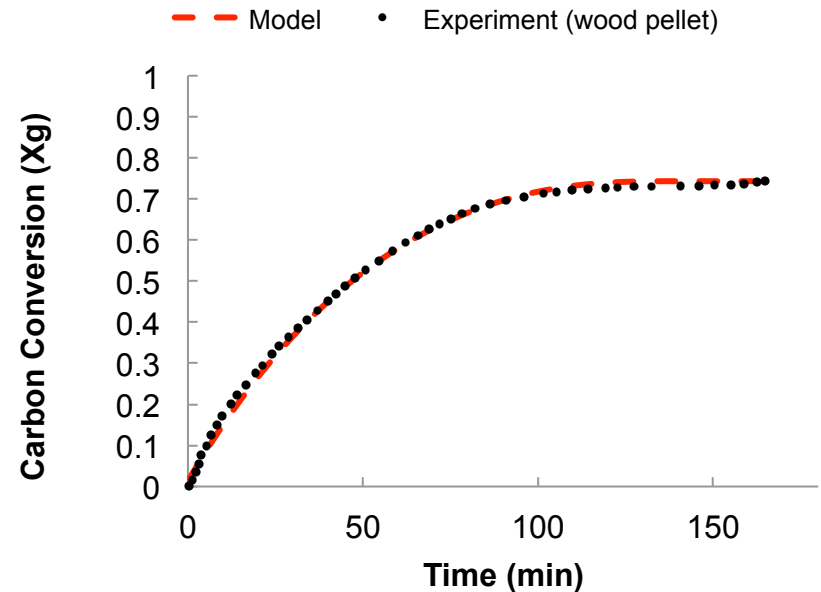
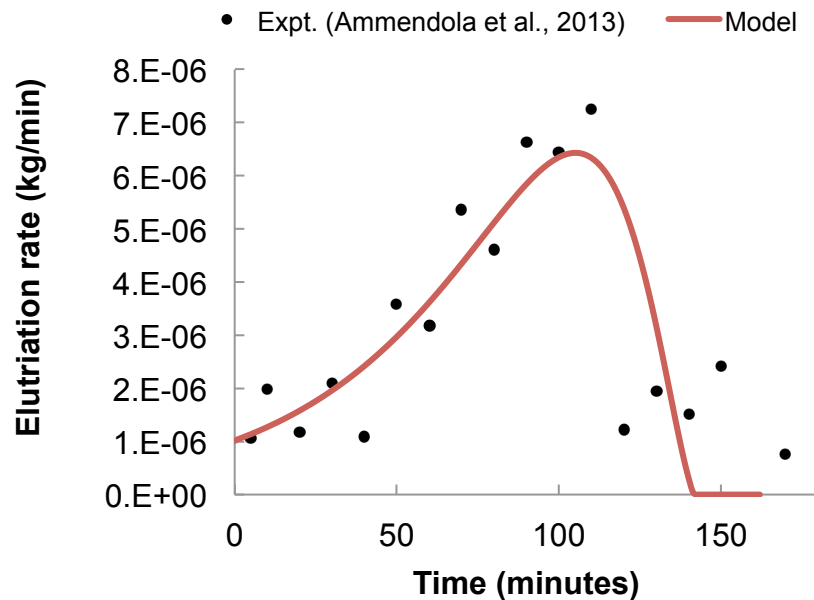


Current model attempts to account for this



Fitted model results:

Spruce wood pellet char gasification in 60%vol CO₂ 800C



- Proposed structural model able to accurately fit results for attrition rate and overall conversion.
- ~25%wt of initial char is attrited over the course of 180 minutes

“Shrinking core model” for char combustion; Internal and external diffusion limitations

$$\eta_{int} = \frac{1}{\phi} \left(\frac{1}{\tanh(3\phi)} - \frac{1}{3\phi} \right)$$

Where

$$\gamma = \sqrt{\frac{kC_c\lambda}{D_e}}, \phi = \frac{\gamma R}{3}$$

Combining external mass transfer limitations the overall rate can be written generally,

$$r_{eff} \left[\frac{\text{mol}_{O_2}}{\text{m}^3_{\text{particle}} \text{sec}} \right] = \frac{C_b}{\frac{d_p}{6} \left(\frac{1}{h_m} + \frac{6}{d_p D_e \gamma^2 \eta} \right)}$$

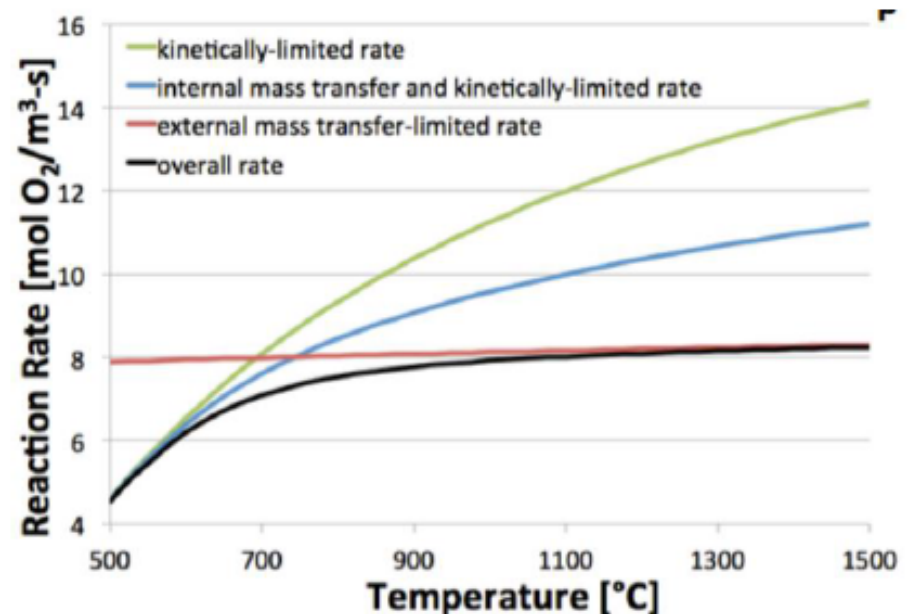
where

$C_c \left[\frac{\text{mol}_{O_2}}{\text{m}^3} \right]$ = concentration of oxygen in the bulk

$D_{eff} \left[\frac{\text{m}^2}{\text{s}} \right]$ = mass diffusivity of oxygen in the porous medium

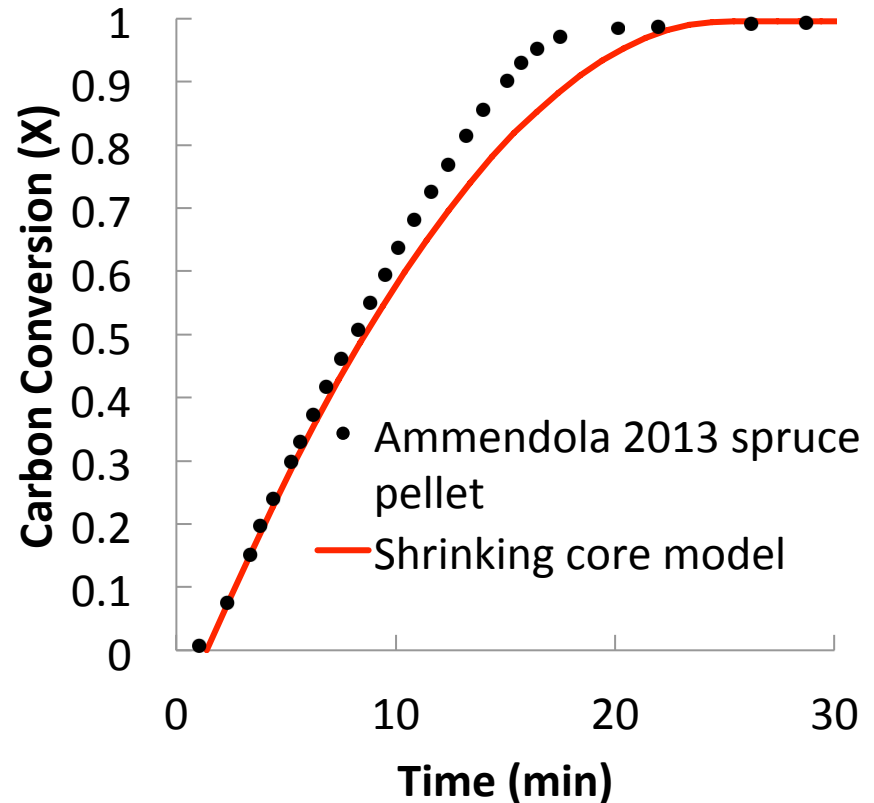
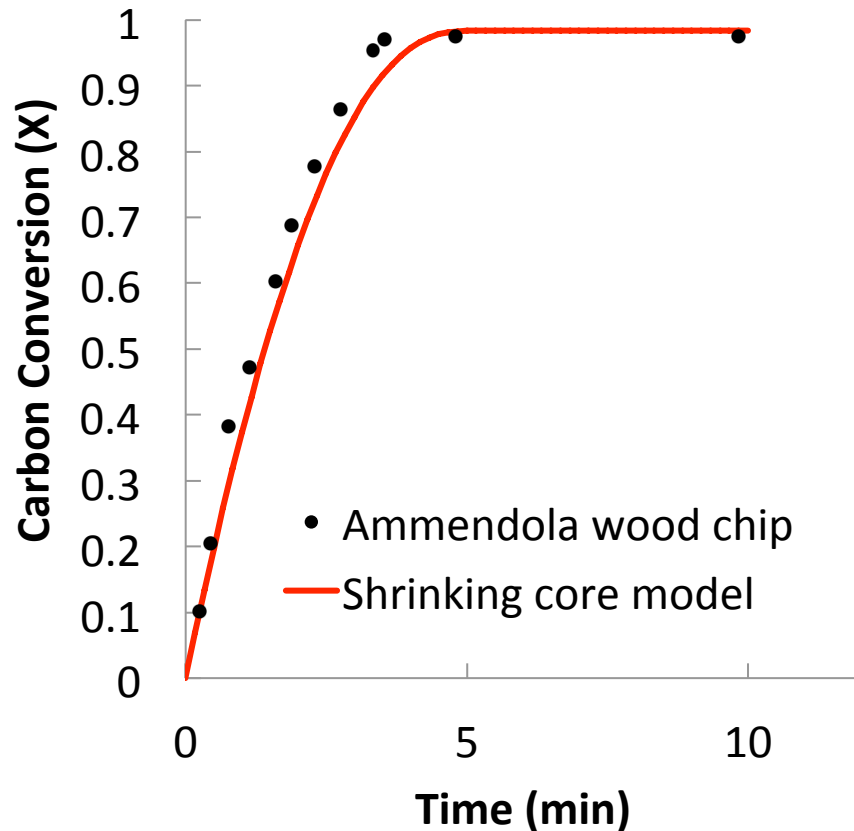
$h_m \left[\frac{\text{m}}{\text{s}} \right]$ = external mass transfer coefficient of oxygen in boundary layer

Reaction rates for 1mm diameter char particle versus temperature



- External mass transfer resistance is significant
 - Sensitive to Sh correlation
- Internal mass transfer resistance also significant at 700-800C

Validation of combustion/attrition particle model



Conditions

4.5% Oxygen at 800C

95.5% Nitrogen

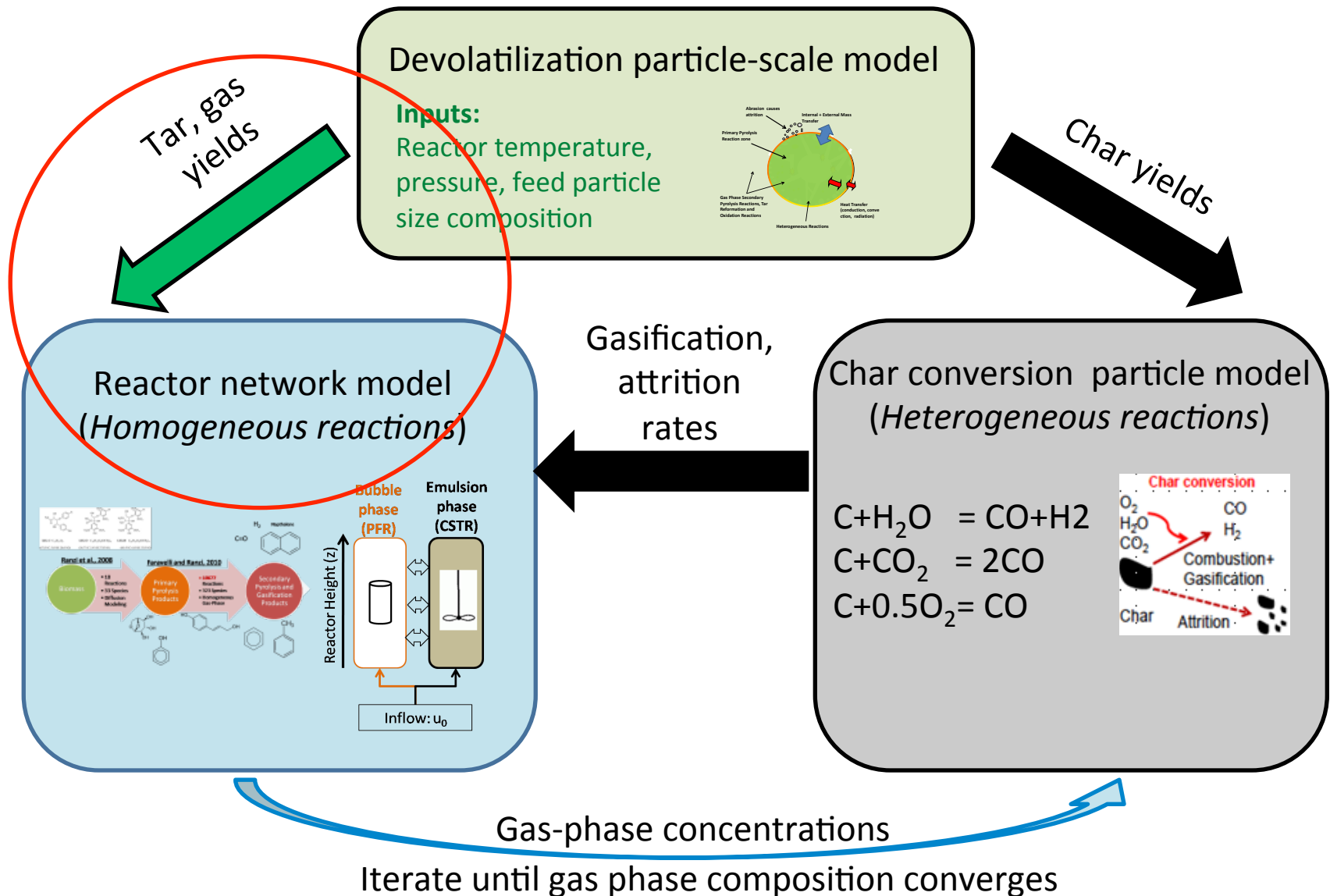
Predictions are sensitive to:

- Particle geometry/aspect ratio
- External mass transfer coefficient
- Char particle density and diffusivity

Char gasification/combustion particle model

- Gasification assisted attrition well represented by new model
 - Sensitive to assumed gasification kinetics
- Combustion for different feedstocks is well represented by effectiveness factor model
 - Rate is sensitive to particle shape and size
 - Sensitive to external mass transfer coefficient model
- Can be incorporated in a RNM.
- In CFD it will be part of a Lagrangian description

Approach: Integrated particle/reactor network models to predict gasifier outputs



Importance of tar yields during biomass gasification

Tar classification based on,

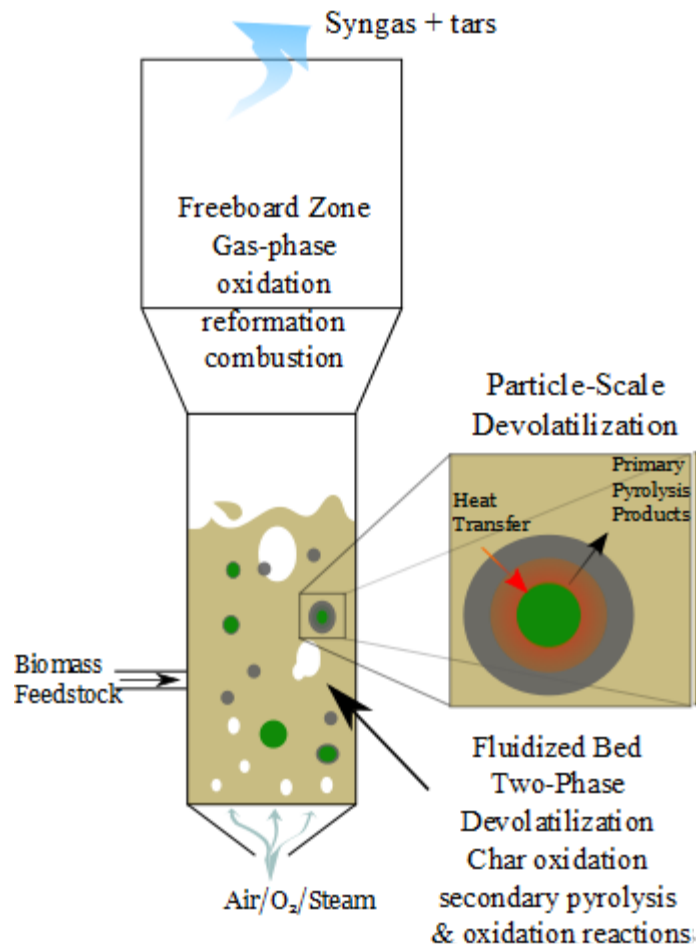
1. Water solubility
2. Condensation temperatures

Downstream problems:

1. Condensation at low temperatures might result in fouling or clogging of the gas pipelines
2. High solubility results in toxic wastewater which would require expensive disposal systems downstream

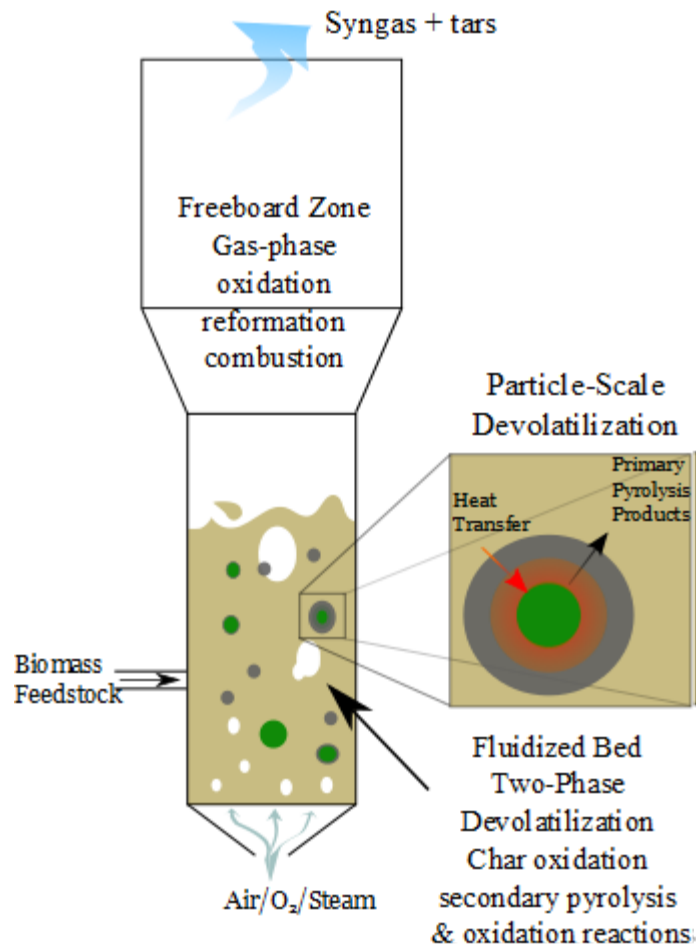
Class #	Species Name	Chemical Formula
Class 1 (GC undetectable)	N/A	N/A
Class 2 (heterocyclic aromatics)	Phenol	C_6H_5OH
	Cresol	C_7H_7OH
	Naphthol	$C_{10}H_7OH$
	Syringol	$C_8H_{10}O_3$
	pCoumaryl	$C_9H_{10}O_2$
	Sinapoyl Aldehyde & isomers	$C_{11}H_{12}O_4$
Class 3 (1-ring aromatics)	Xylene	C_8H_{10}
	Styrene	$C_6H_5C_2H_3$
	toluene	C_7H_8
	Benzene	C_6H_6
Class 4 (light PAH [2-3 ring])	Naphthalene	$C_{10}H_8$
	acenaphthalene+isomers	$C_{12}H_8$
	Biphenyl	$C_{12}H_{10}$
	Fluorene	$C_{13}H_{10}$
	phenanthrene+anthracene	$C_{14}H_{10}$
	benzylphenylmethane	$C_6H_5C_2H_4C_6H_5$
	Diphenylmethane	$C_6H_5CH_2C_6H_5$
Class 5 (heavy PAH [4-7 ring])	pyrene+isomers	$C_{16}H_{10}$
	7,12-Dimethylbenz(a)anthracene & iso.	$C_{20}H_{16}$
	Corannulene and isomers	$C_{20}H_{10}$

Reactor network model of fluidized biomass gasifier

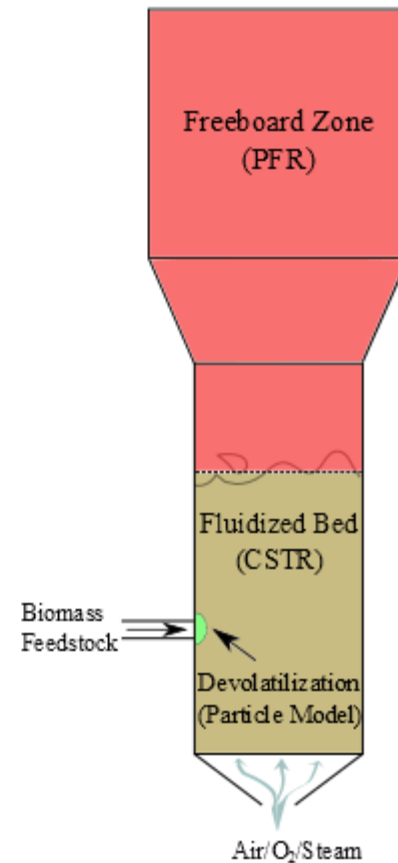


- Fluidized bed is well mixed at rate faster than timescale of devolatilization
 - Devolatilization is uniform through bed
 - Gas-phase reactions in emulsion can be modeled as a CSTR (continuously stirred tank reactor)
- In freeboard few solids present thus little axial mixing
 - Gas-phase reactions in freeboard can be modeled as a PFR (plug flow reactor)

Reactor network model of fluidized biomass gasifier

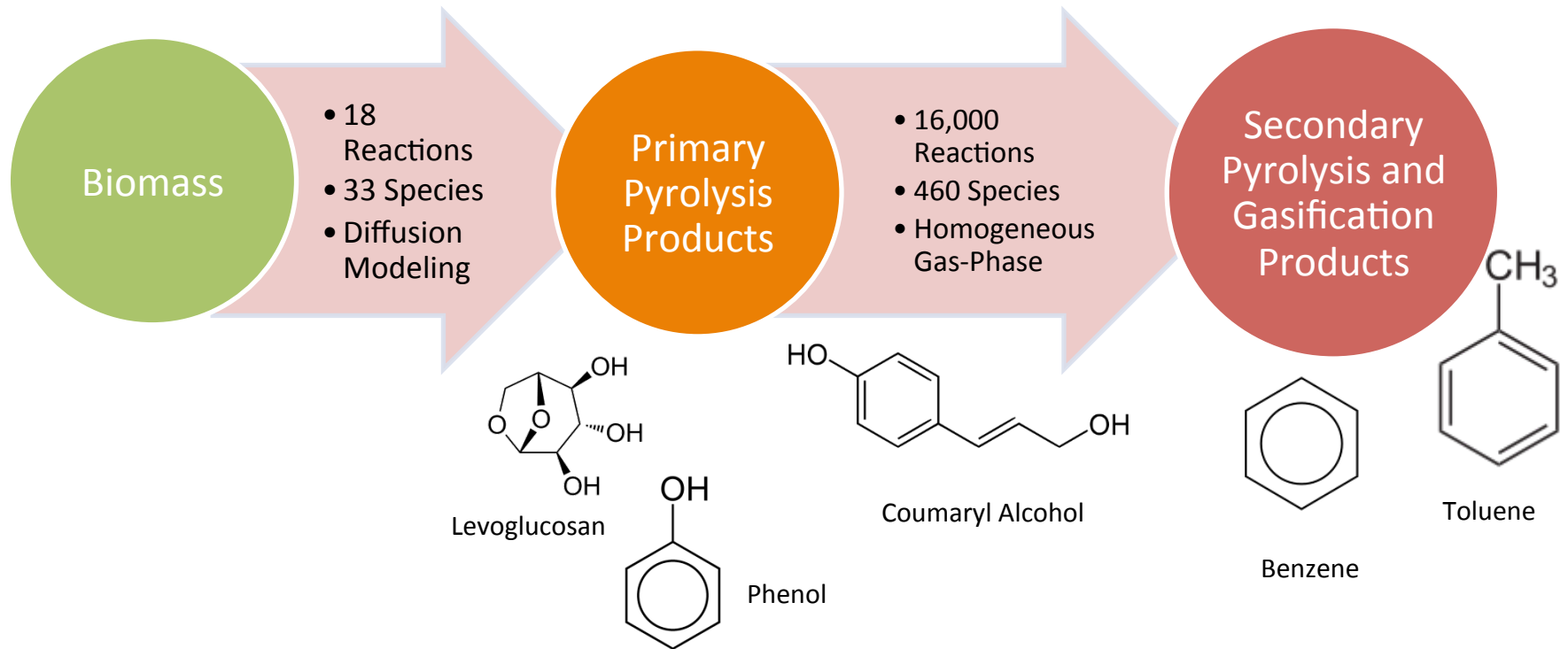
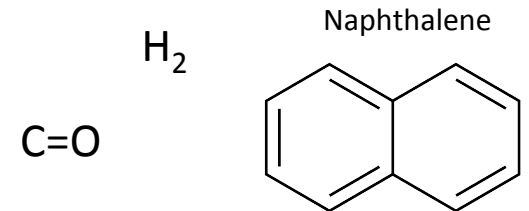
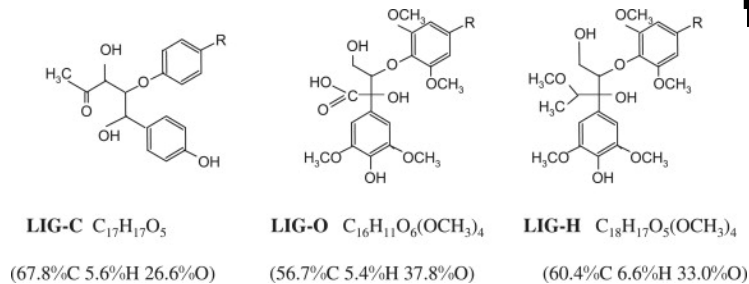


FBG Reactor Modeling Framework

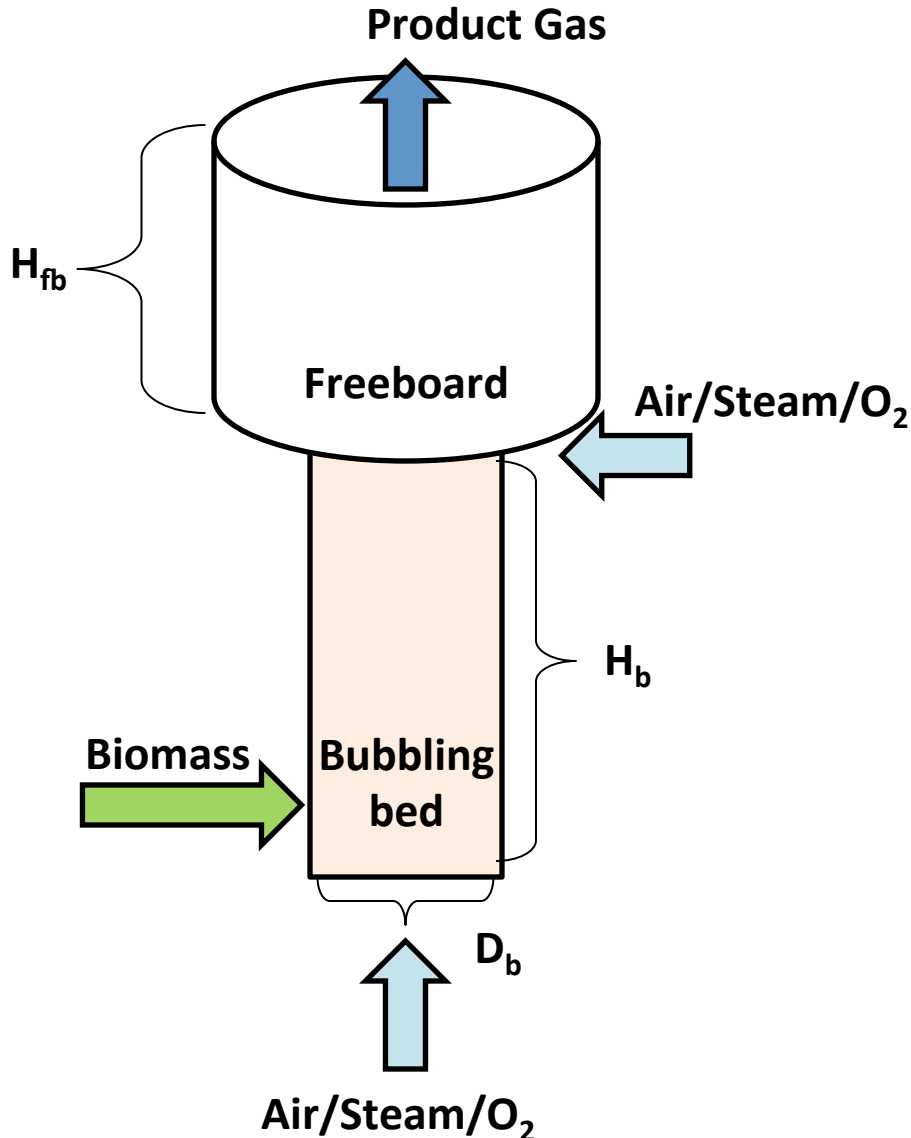


Mechanism:
CRECK/Ranzi
~460 Species
~16000 Reactions

CRECK mechanism for primary pyrolysis and secondary gas phase reactions



Experimental data available for validation: Air-blown bubbling fluidized bed gasifiers.



(Van Paasen and Kiel, 2004 [16])

- Biomass feed rate: 1kg/hr
- Biomass feedstock: Beech
- Air-Fuel Equivalence Ratio: 0.25
- Fluidizing medium: Sand, 270 μm micron
- Bed diameter= 7.4 cm

(Narvaez et al., 1996 [17])

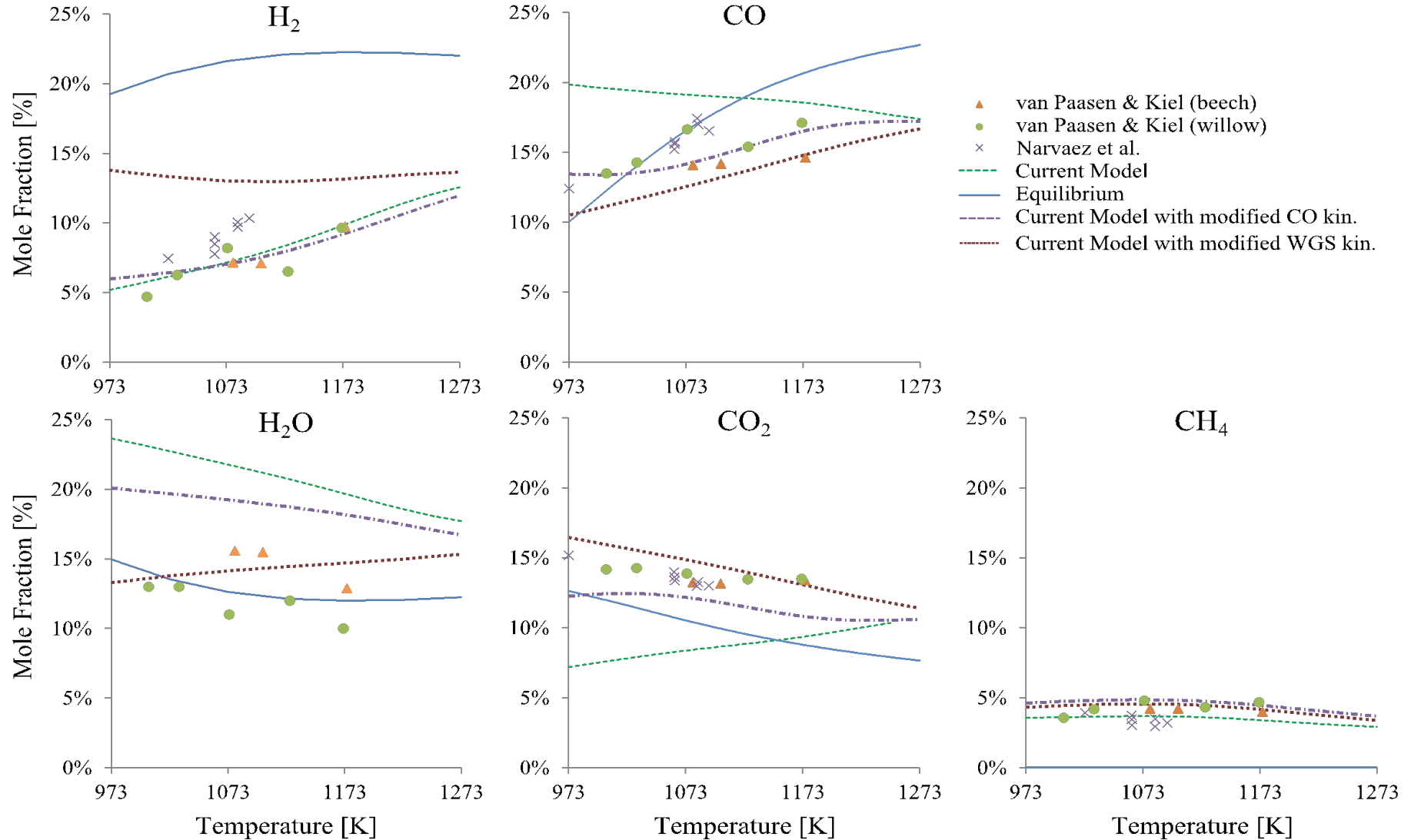
- Biomass feed rate: 0.5kg/hr
- Biomass feedstock: Pine sawdust
- Air-Fuel Equivalence Ratio: 0.25-0.4
- Fluidizing medium: Sand, 360 μm
- Bed diameter=6 cm

(Kurkela & Stahlberg, 1992 [18])

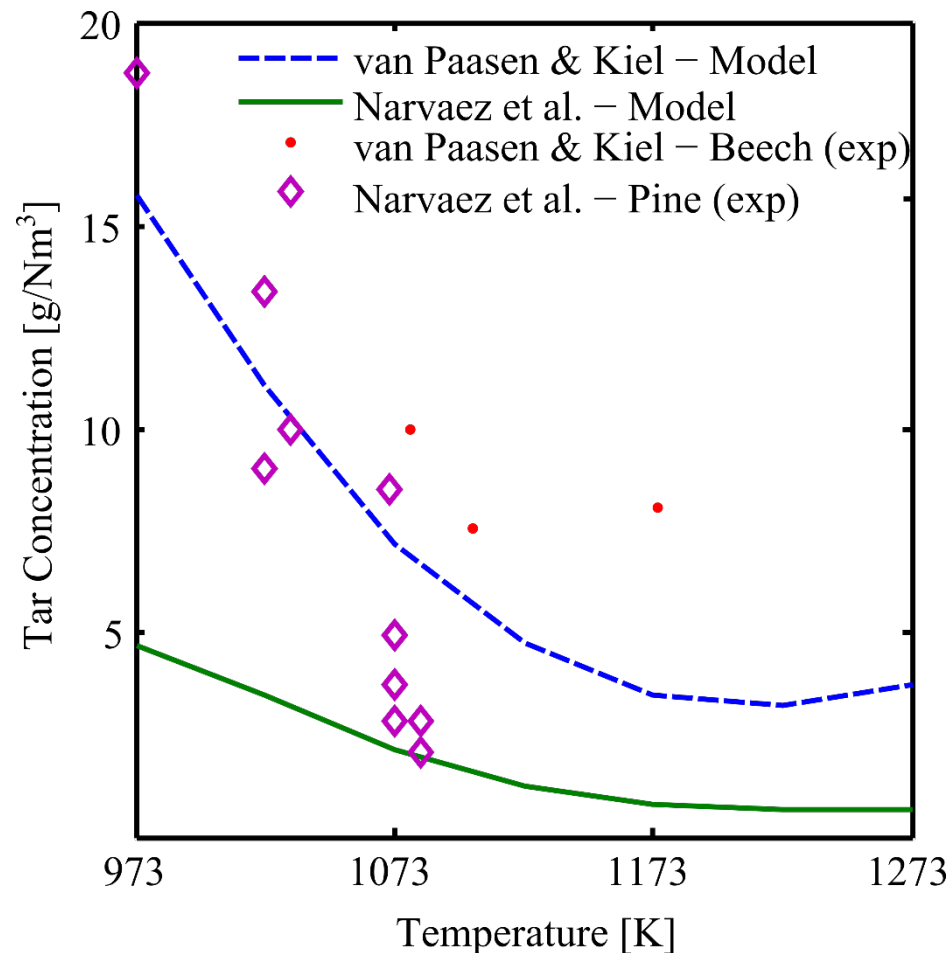
- Biomass feed rate: 40kg/hr
- Biomass feedstock: Pine sawdust
- Air and Steam employed
- Air-Fuel Equivalence Ratio: 0.25-0.4
- Fluidizing medium: Sand, 600 μm
- Bed diameter=15 cm
- At pressure (4 bar)
- Secondary Air injection.

RNM validation:

Effects of temperature on major species, effects of CO and Water Gas Shift Kinetics.

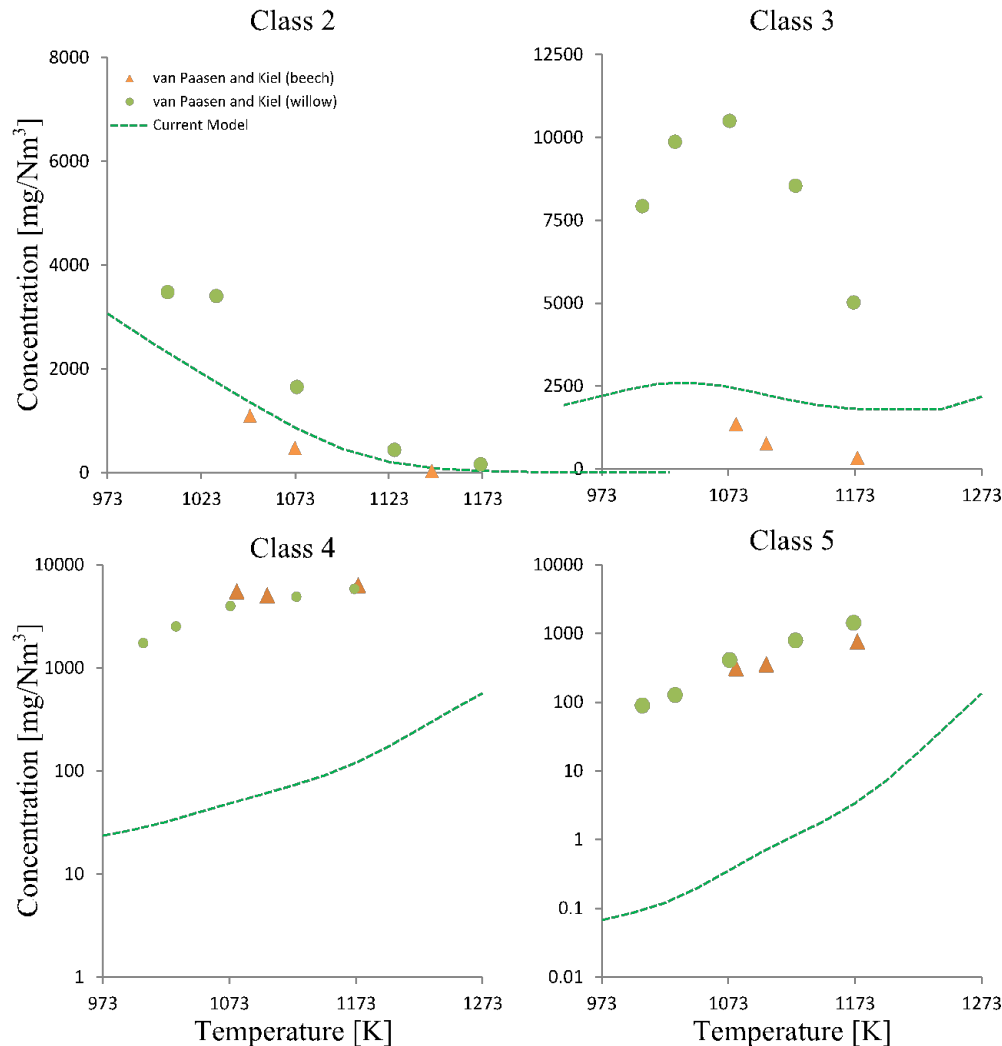


Comparison of full mechanism with experimental data



- Full mechanism and reactor network model able to accurately represent the destruction of tars at higher temperatures

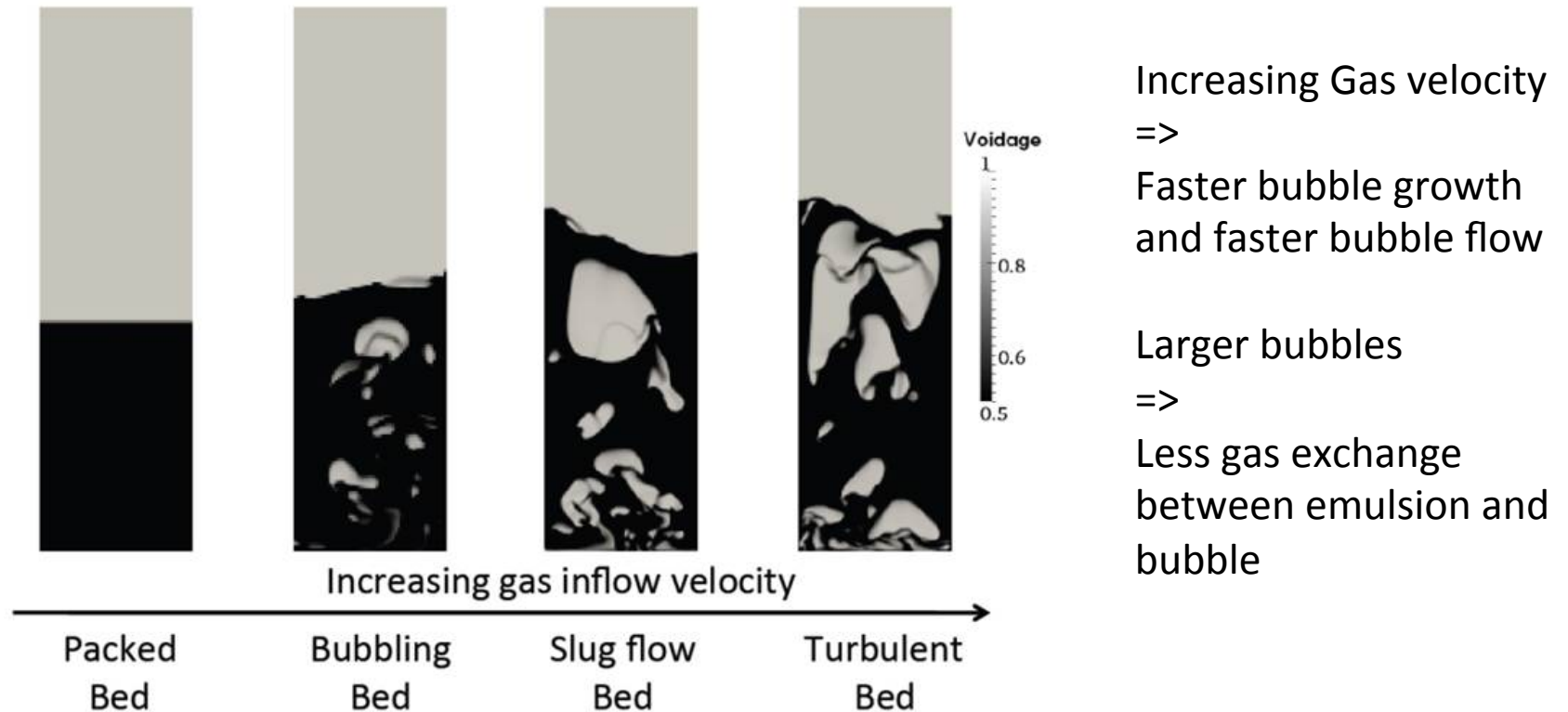
Tar Class predictions



We are under-predicting the formation of PAH compounds... by orders of magnitude

Well Stirred bed possibly over-predicts availability of oxygen everywhere, impeding PAH formation... Transport likely playing a role!

Well-stirred Bed Zone is a strong assumption



Increasing Gas velocity

=>

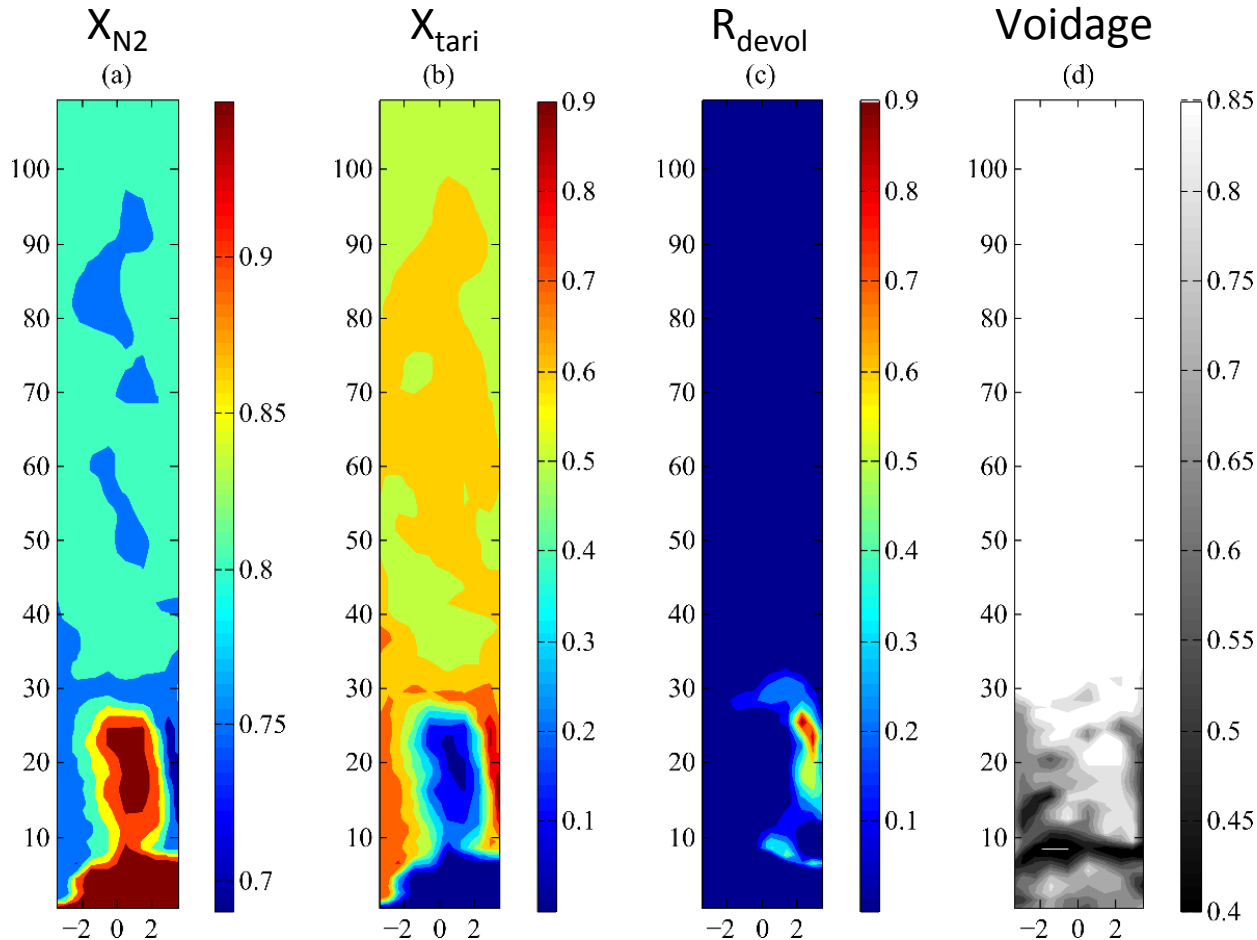
Faster bubble growth
and faster bubble flow

Larger bubbles

=>

Less gas exchange
between emulsion and
bubble

Well-stirred Bed Zone is a strong assumption

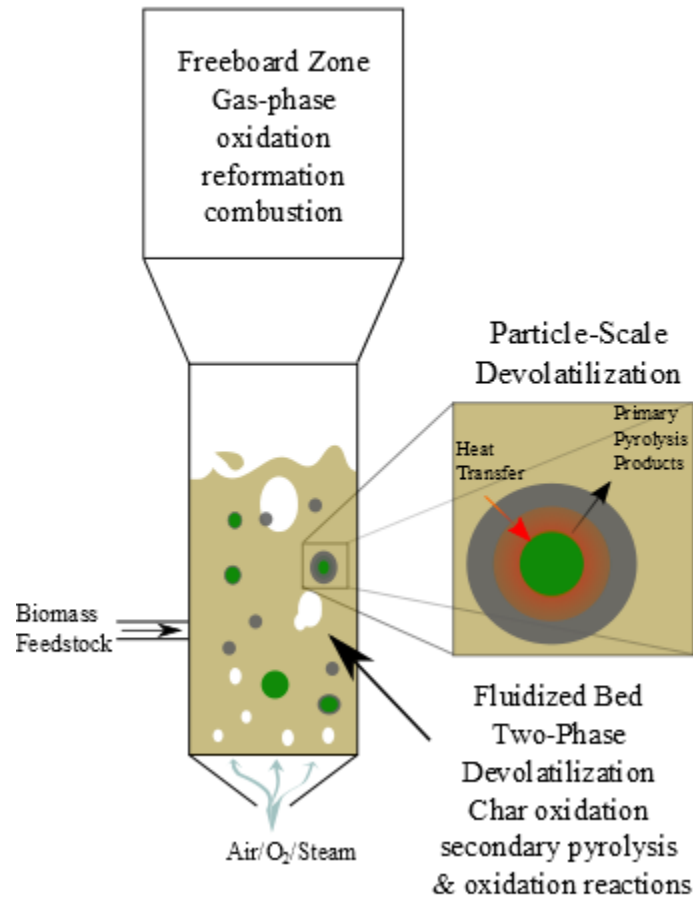


- Bubbles carry majority of excess fluidization gas
- Devolatilization occurs in emulsion
- Full mixing occurs at splash zone
- Emulsion relatively rich...

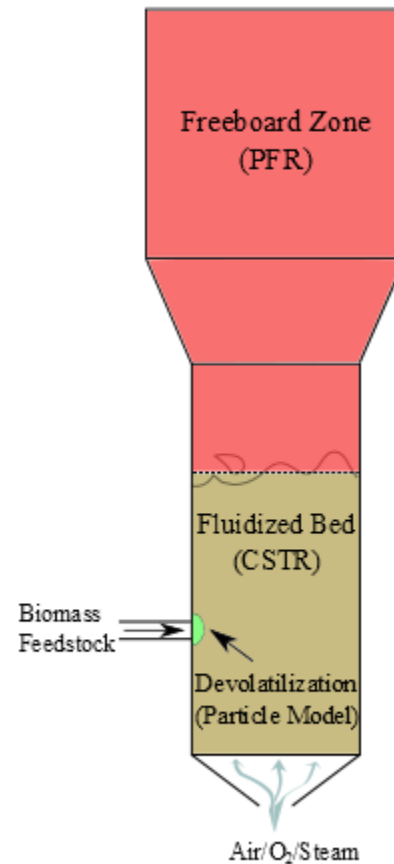
RNM needs to capture this to predict PAH formation.

Improved RNM Formulation

Chemical Processes in FBG

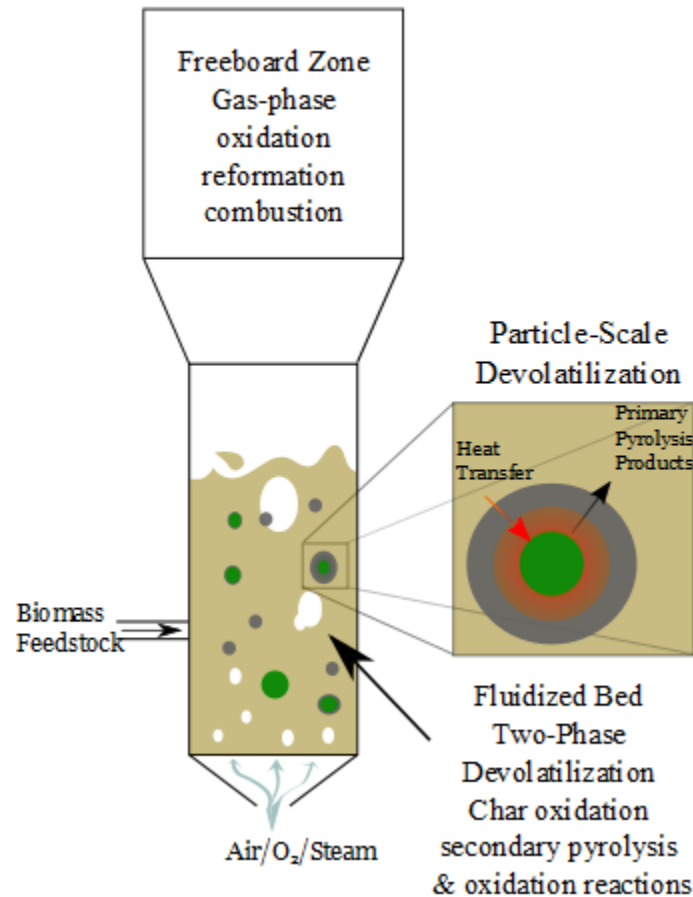


FBG Reactor Modeling Framework

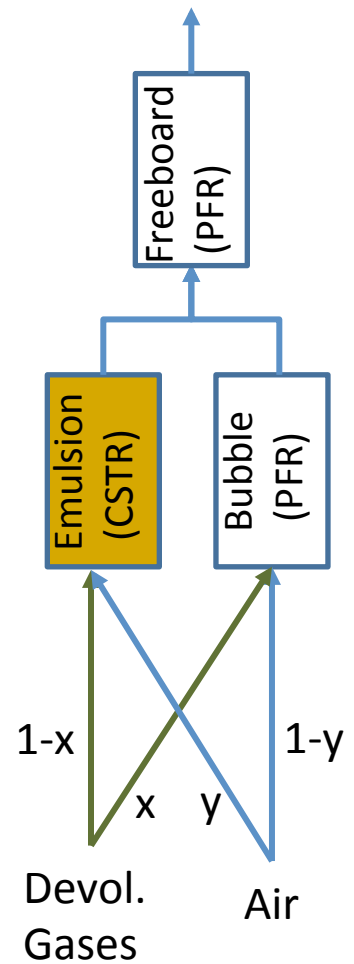
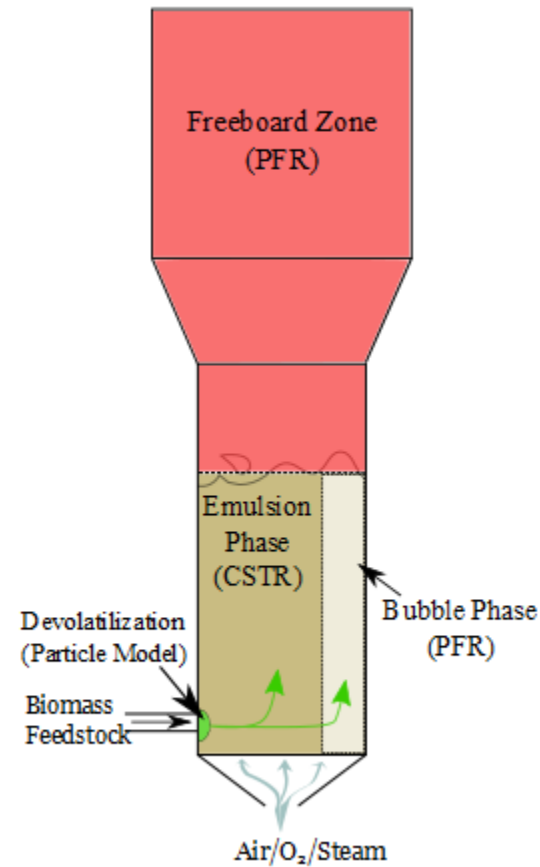


Improved RNM Formulation

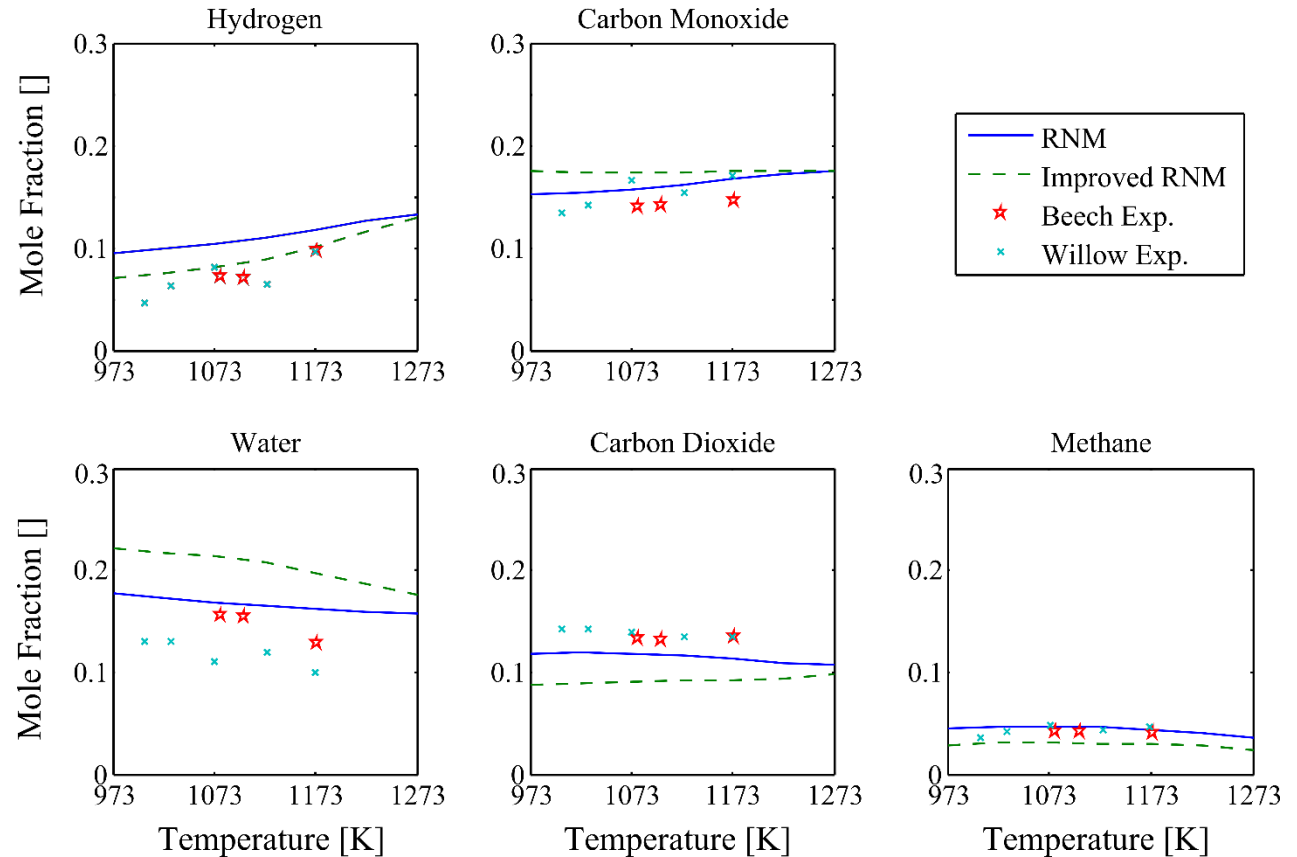
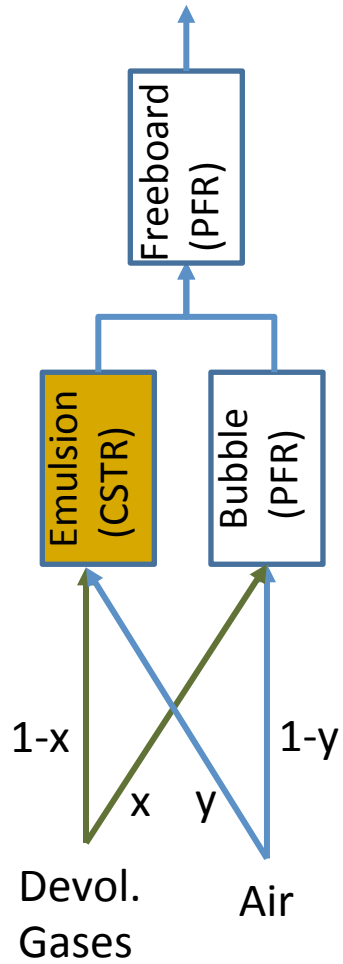
Chemical Processes in FBG



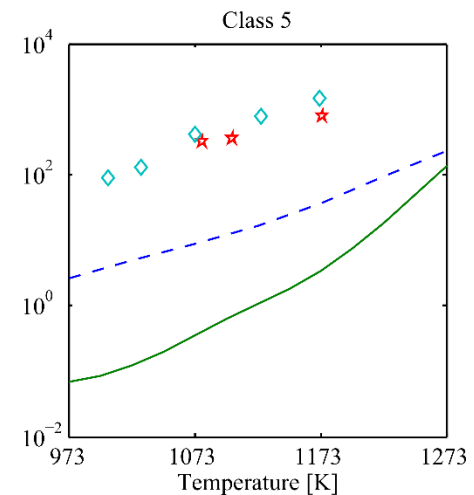
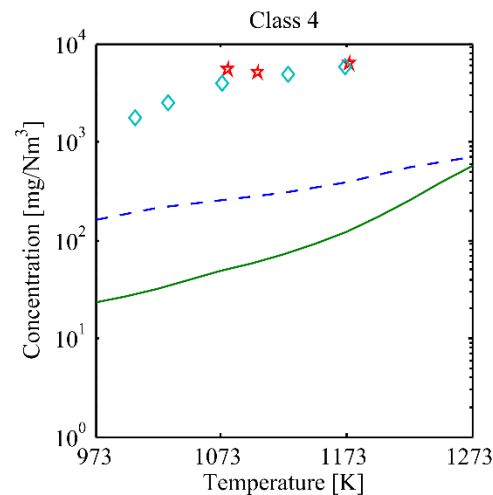
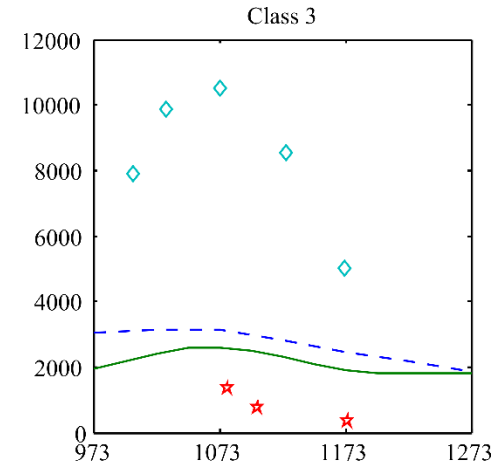
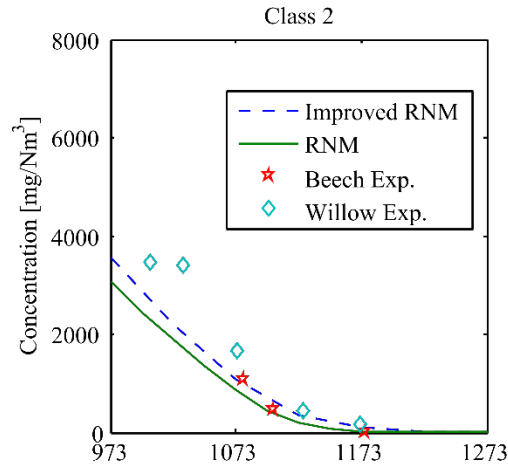
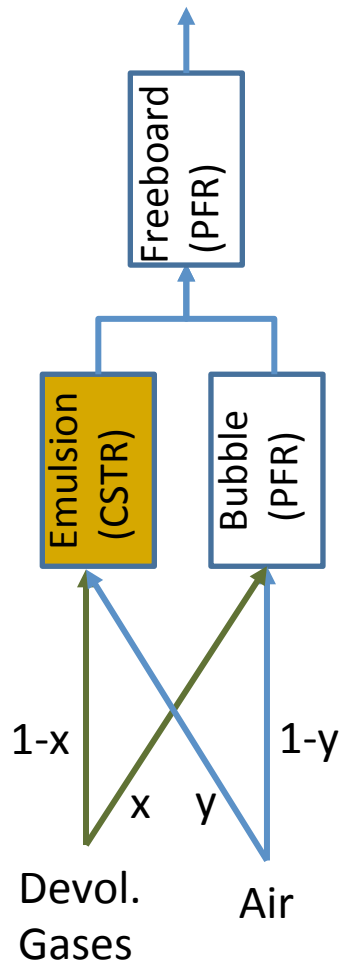
FBG Reactor Modeling Framework



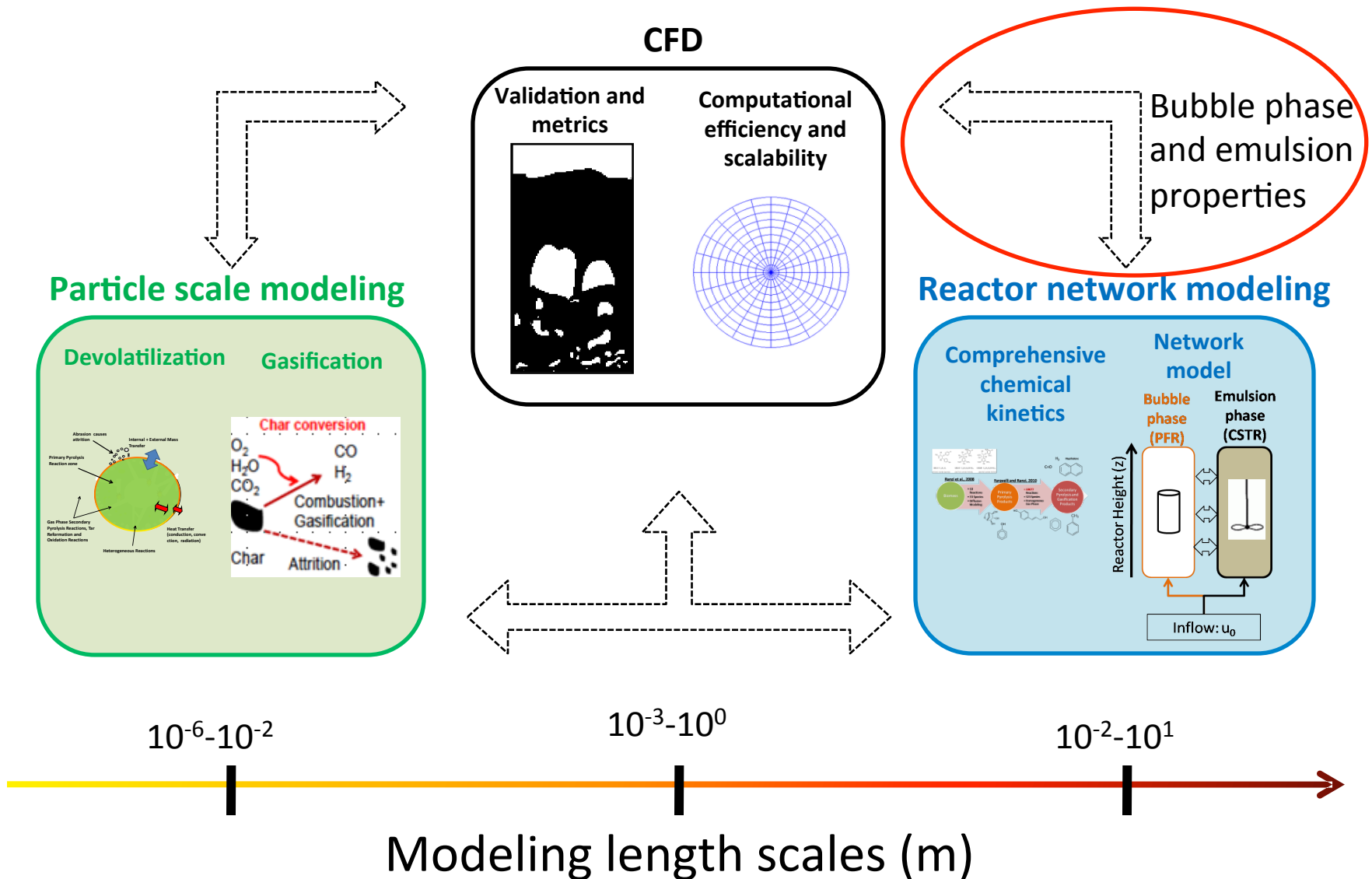
Impact of bubble-phase on gas-phase conversion



Impact of bubble-phase on gas-phase conversion



Current work: Coupling CFD, particle thermochemistry and RNM



Concluding remarks

- Multi-scale simulation necessary to tackle the complexity of fluidized bed biomass gasification
- Eulerian Eulerian approach for fluidization offers computational scalability but requires closures and validation
 - Contributions in appropriate metrics, robust parametrization, computational efficiency
- Particle scale modeling:
 - FBG dominated by particle scale processes of devolatilization, gasification and combustion
 - Dominant physical/chemical processes must be identified
 - Impossible to model “all” processes
- Reactor network modeling
 - Flexible, incorporates comprehensive chemistry and particle models
 - Can benefit from CFD results (gas distribution, exchange ...)

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