Mass Transfer Effects in a Gasification Riser

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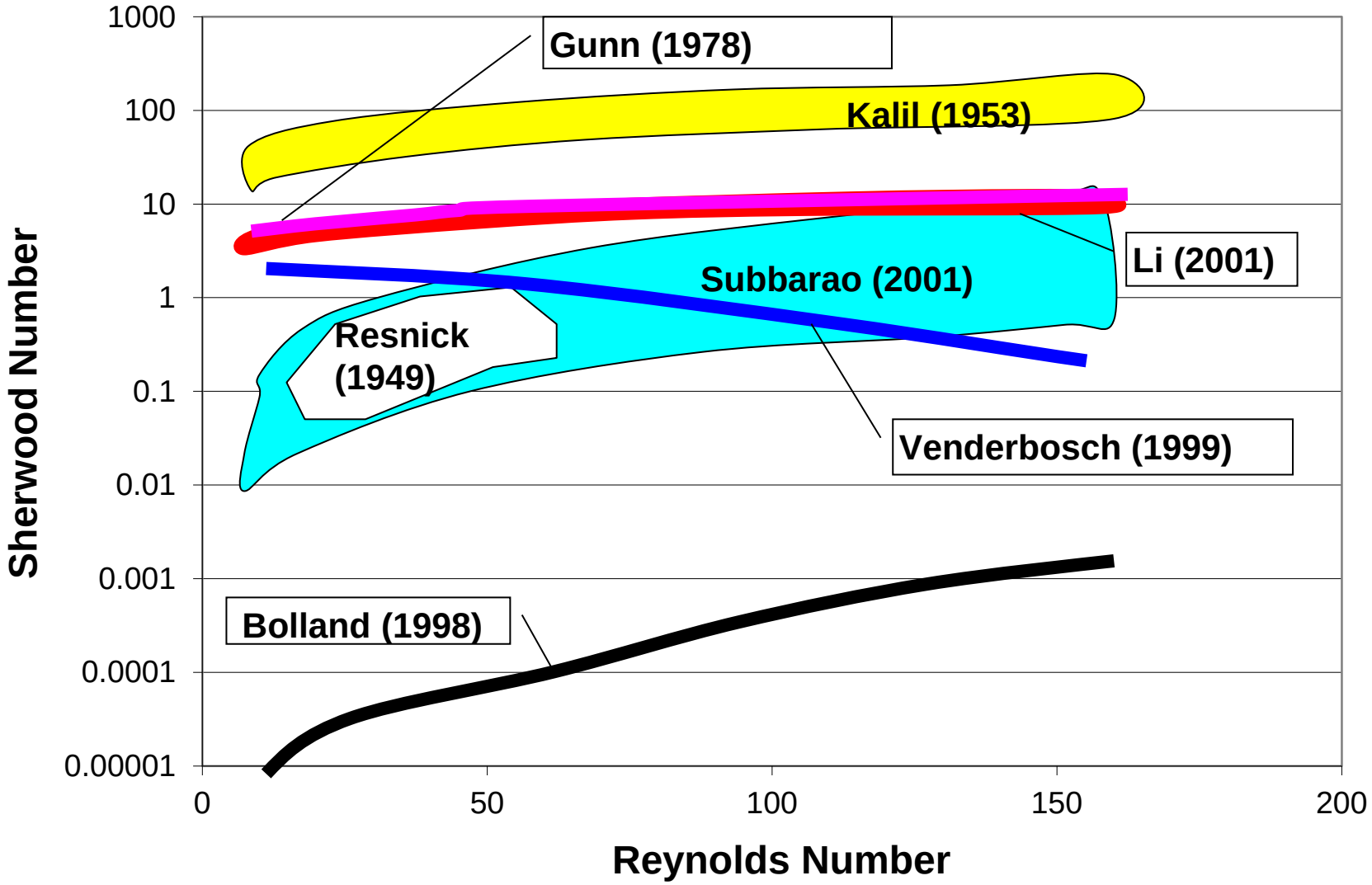
Background

- In the development of multiphase reacting CFD codes, a number of simplifications were incorporated into the codes and models.
- One of these simplifications was the use of a simplistic mass transfer correlation for the faster reactions and omission of mass transfer effects completely on the moderate speed and slow speed reactions such as those in a fluidized bed gasifier.
- Another problem that has propagated is that the mass transfer correlation used in the codes is not universal and is being used far from its developed bubbling fluidized bed regime when applied to riser reactors.
- These problems are true for all the major codes: Fluent and MFIX/C3M as well as for Barracuda.

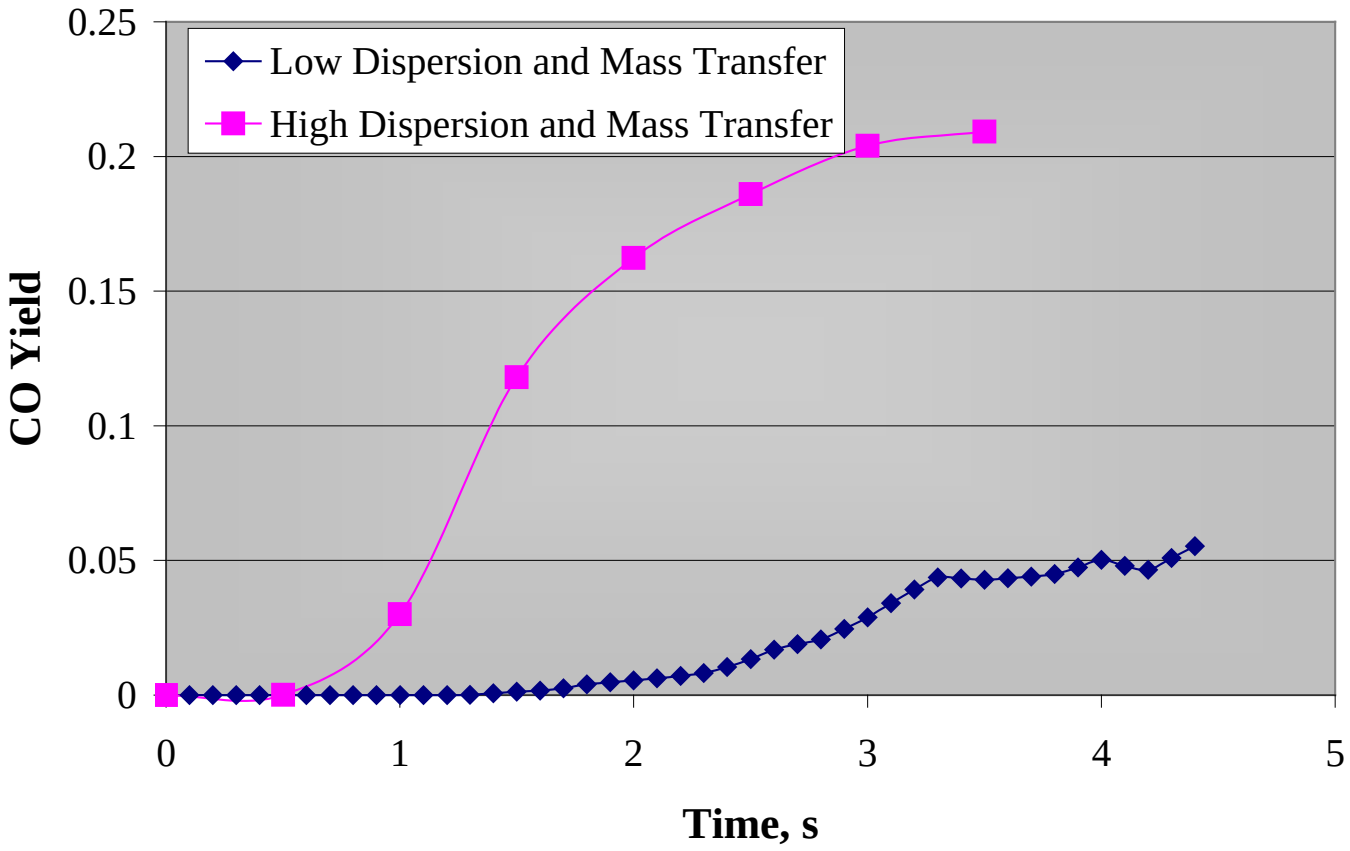
Aspects of Mass Transfer

- **Convective mass transfer – modeled using mass transfer coefficient or Sherwood Number correlations**
- **Turbulent dispersion/diffusion – the propagation of a reacting species through the reactor due to turbulent eddy pocket movements**

Mass Transfer in CFB Conditions

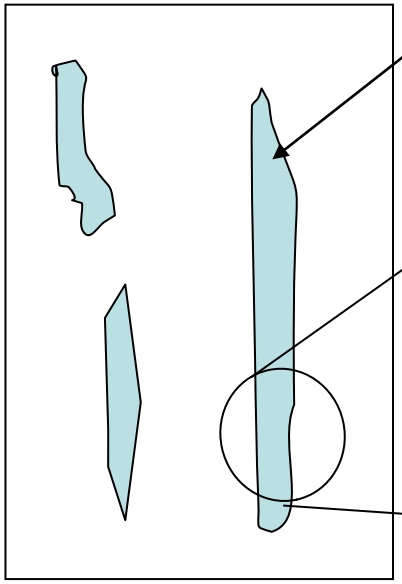


Effect of Transport Properties on MFIX Simulation of Industrial Scale CFB Coal Partial Oxidizer

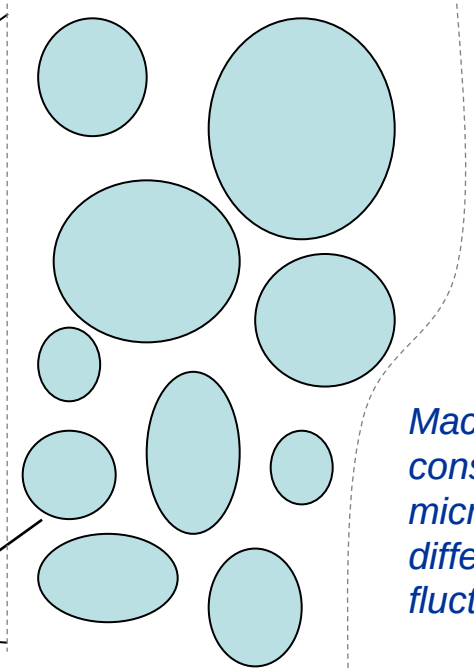


Mass Transfer in Clustering Flows

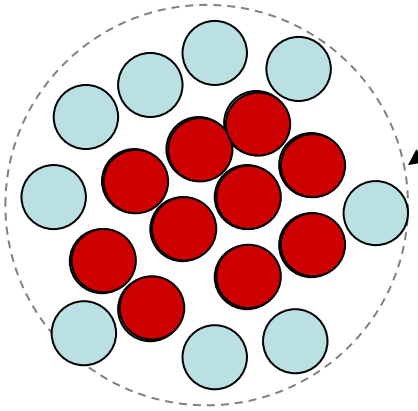
Riser section with clusters containing reactive species for gas-solids reaction



Macro-clusters on the size of the equipment

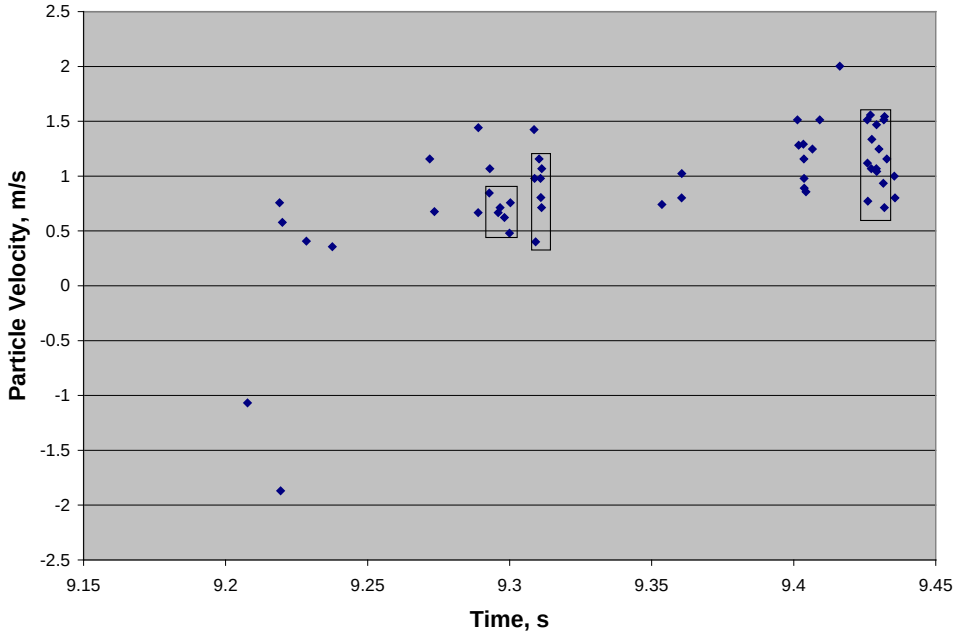


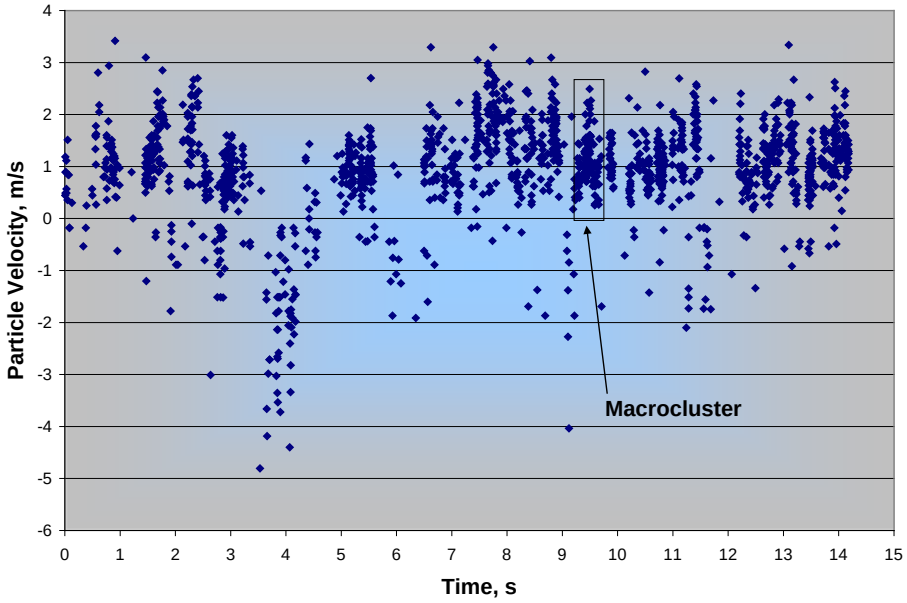
Macro-cluster consists of many micro-clusters of different size and fluctuating energy



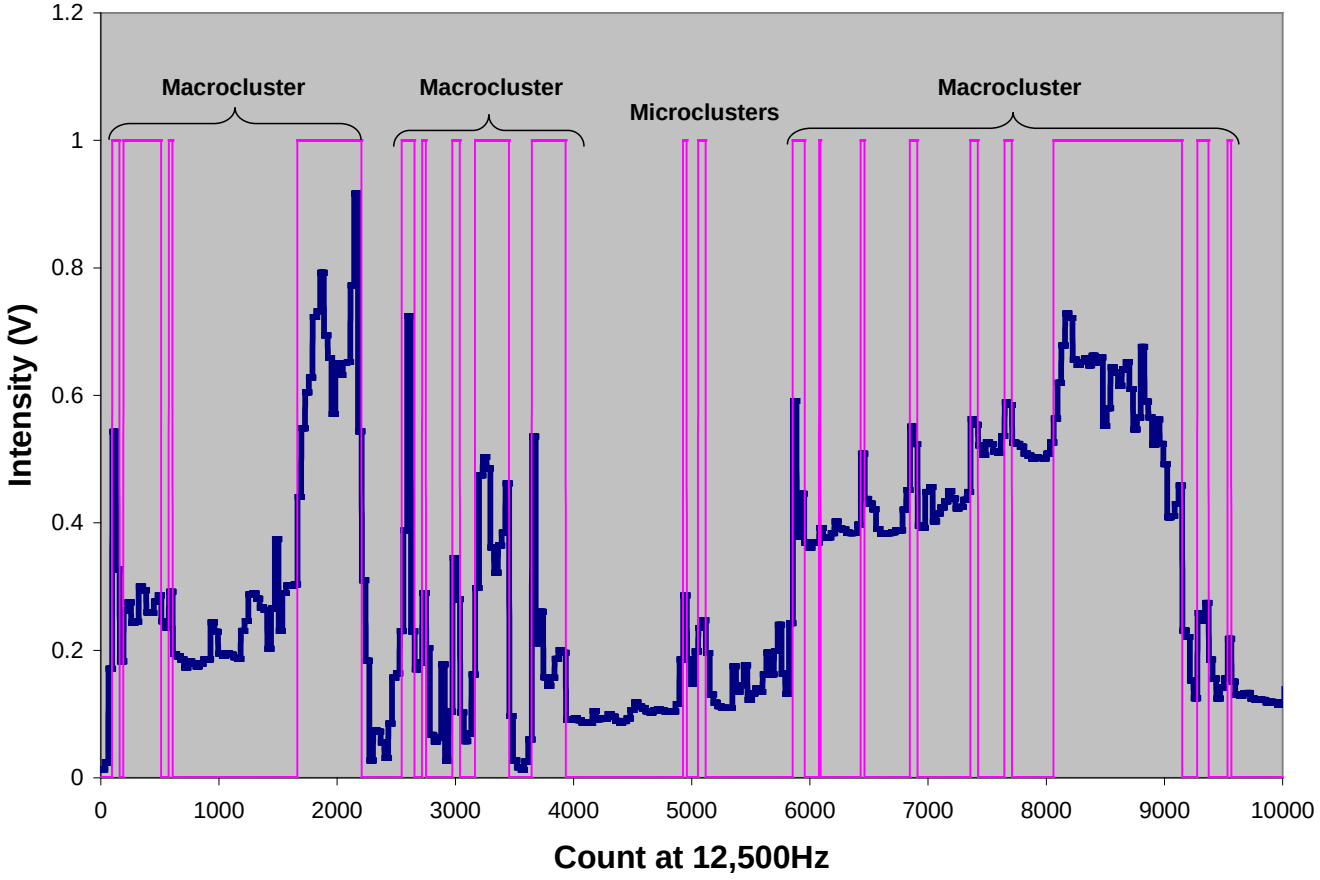
How is mass or heat for transferred from the gas to the solid in the center of the cluster?

Micro and Macro Clusters from LDV

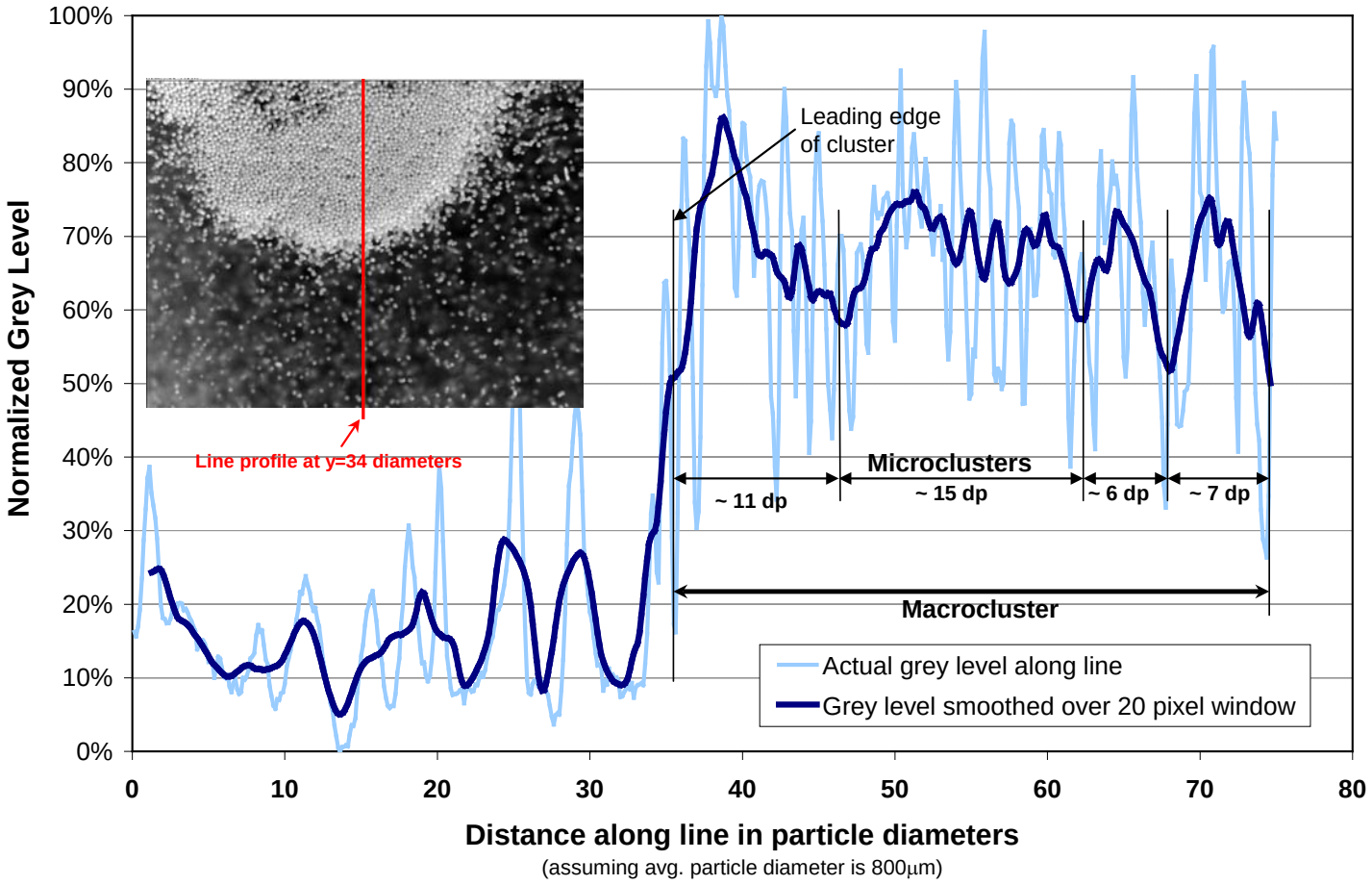




Micro and Macro Clusters from Fiber Optic Data

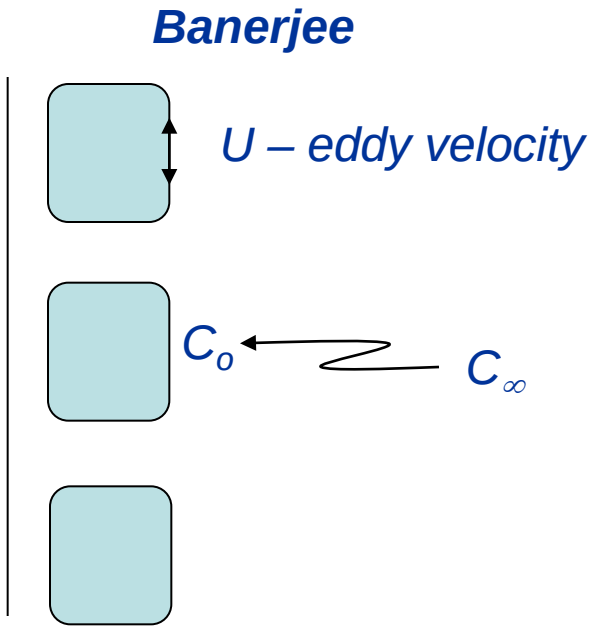


Micro and Macro Clusters from Advanced Imaging



Mass Transfer Analogies

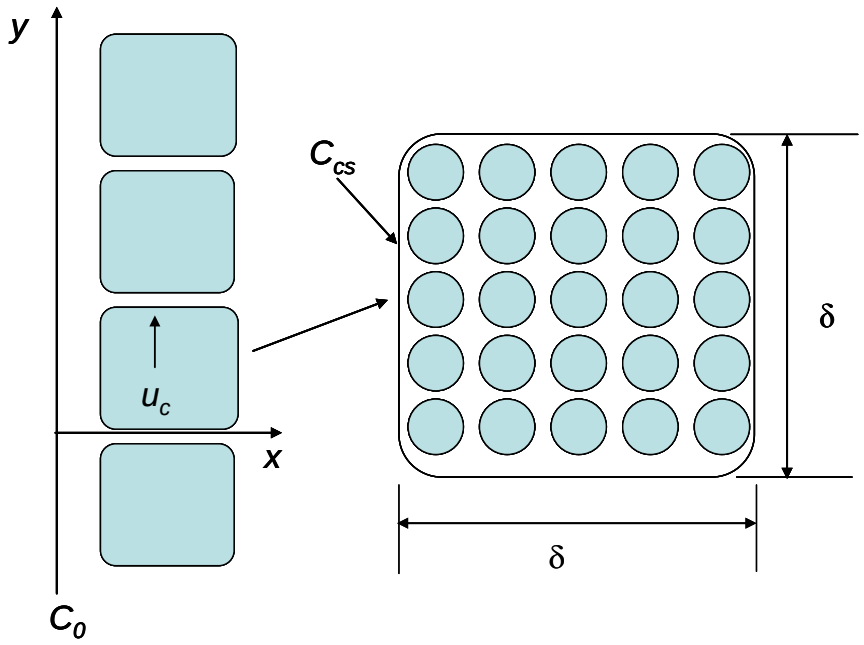
- **Penetration theory (Higbie in 1935)**
- **Penetration theory with random surface renewal (Dancwerts in 1951)**
- **Film-penetration theory (Toor an Machello in 1958)**
- **Transfer to falling turbulent wavy films (Banerjee, Scott and Rhodes in 1968)**



$$k \approx \sqrt{\frac{4D}{\pi\ t_e}} \approx \sqrt{sD} \approx \sqrt{\frac{4Du}{\pi\ \delta}}$$

$$\frac{1}{t_e} = \frac{u}{\delta} \cong s$$

Clustering Flow Model



$$u_c \frac{\partial \overline{C}}{\partial y} = D \frac{\partial^2 \overline{C}}{\partial x^2}$$

$$\overline{C} = \frac{C - C_{cs}}{C_0 - C_{cs}}$$

$$y = 0, \quad \overline{C} = 0$$

$$x = 0, \quad \overline{C} = 1$$

$$x = \delta, \quad \overline{C} = 0$$

Solution

The solution of this equation can be found in a number of textbooks, for example see Bird, Stewart and Lightfoot .

$$\overline{C} = 1 - erf \frac{x}{\sqrt{4Dy / u_c}}$$

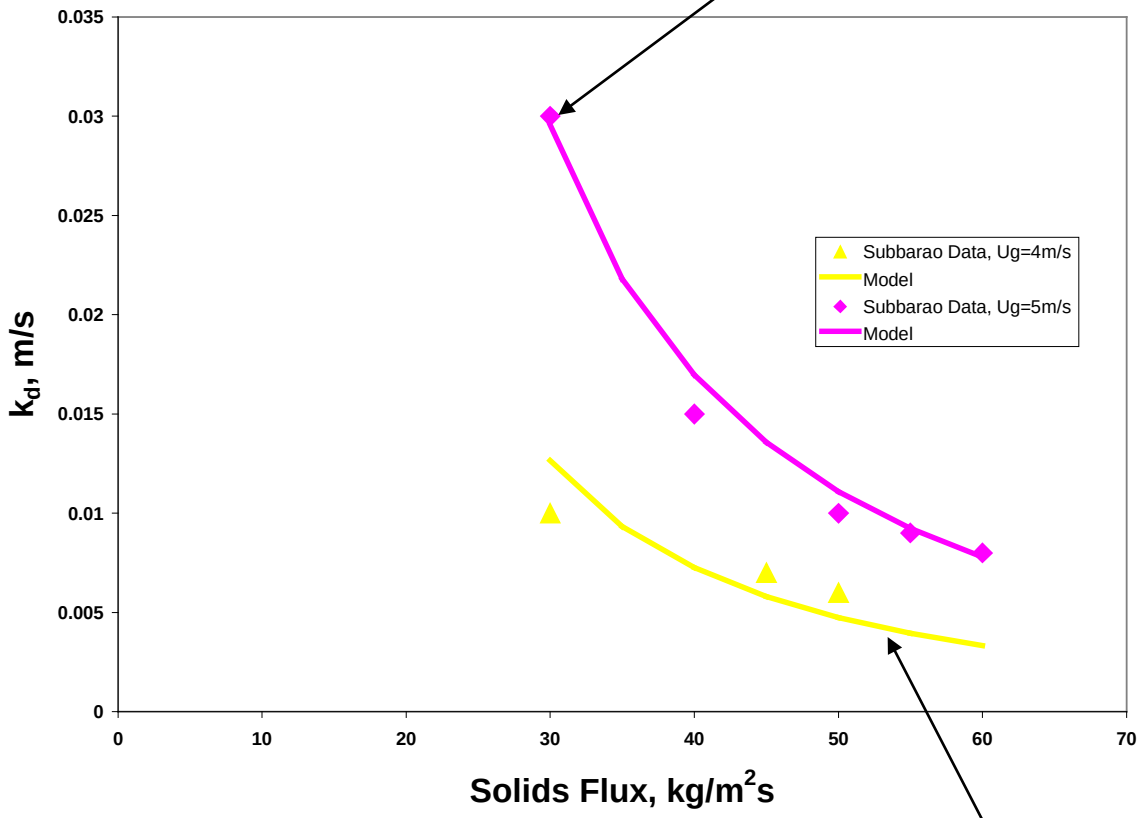
$$k = \sqrt{\frac{4Du_c}{\pi\delta}}$$

$$k = \sqrt{\frac{4D\sqrt{(u_c)^2}}{\pi\delta}}$$

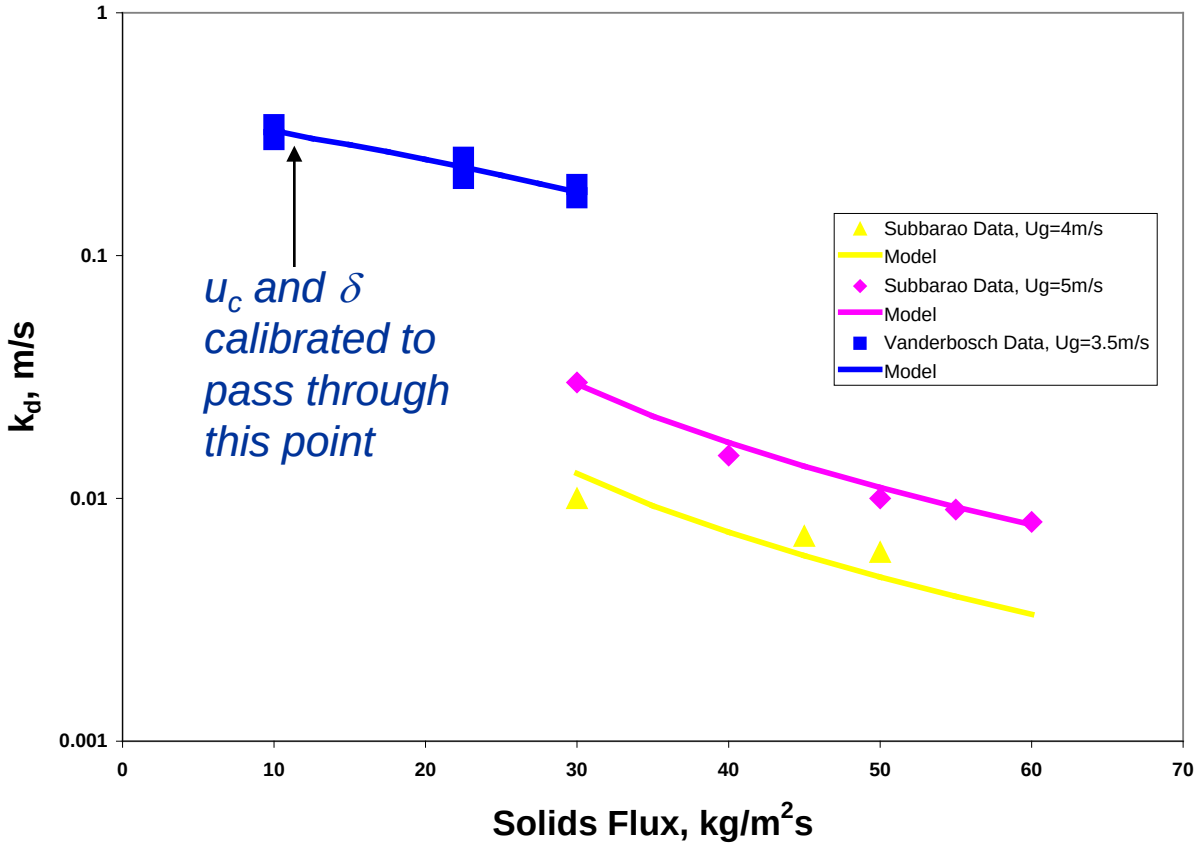
Mass Transfer Coefficient, m/s

Experimental		Theory (Equation 8)	
Value	Error	Value	Error
0.010	±.002	0.012	+0.0004, -0.001
0.015	±.003	0.014	+0.0008, -0.001

u_c and δ calibrated to pass through this point



Cluster dynamics assumed to behave the similar to cork in the CFTF with changes in solids and gas flow rates


1
0.1
0.01
0.001
k_d, m/s
0
10
20
30
40
50
60
70
Solids Flux, kg/m^{2}s
u_c and δ calibrated to pass through this point
Subbarao Data, Ug=4m/s
Model
Subbarao Data, Ug=5m/s
Model
Vanderbosch Data, Ug=3.5m/s
Model

Model as Installed in Baseline Code

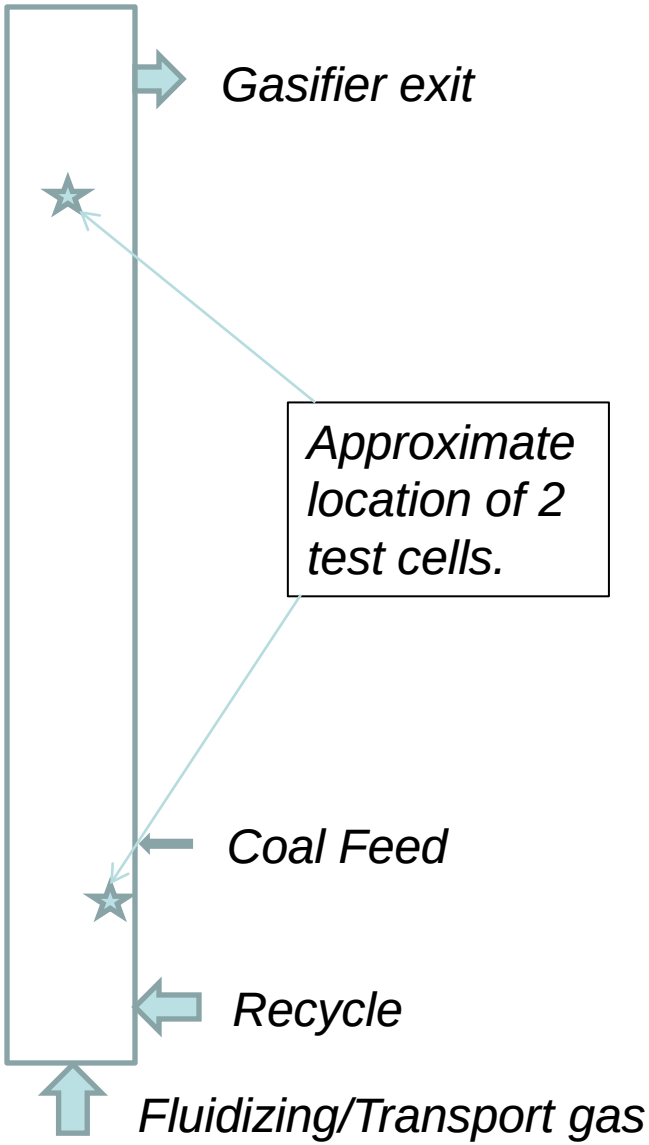
- To effectively calculate the mass transfer coefficient according to the model presented, the cluster size and the cluster fluctuating energy is required in each cell.
  - Based upon the work of Breault, Ludlow and Yue, clusters are small groups of particles moving in the same direction, being separated from one another by as much as one particle diameter and having similar granular temperature to its neighboring particles.
  - Breault showed elsewhere that there is a distribution of cluster sizes in the riser ranging from six to 10 particle diameters on the small end to +20 cm on the high end.
  - Due to the transient nature of the code, with each time step, each and every cell contains a different quantity of particles, it is therefore proposed to have the cluster size calculated from the following equation, taking clusters to be at a packing equal to that of minimum fluidization.

$$\delta = \left(\frac{6\varepsilon_s}{\pi \varepsilon_{mf}} V_{cell} \right)^{1/3}$$

Simulation Input Data

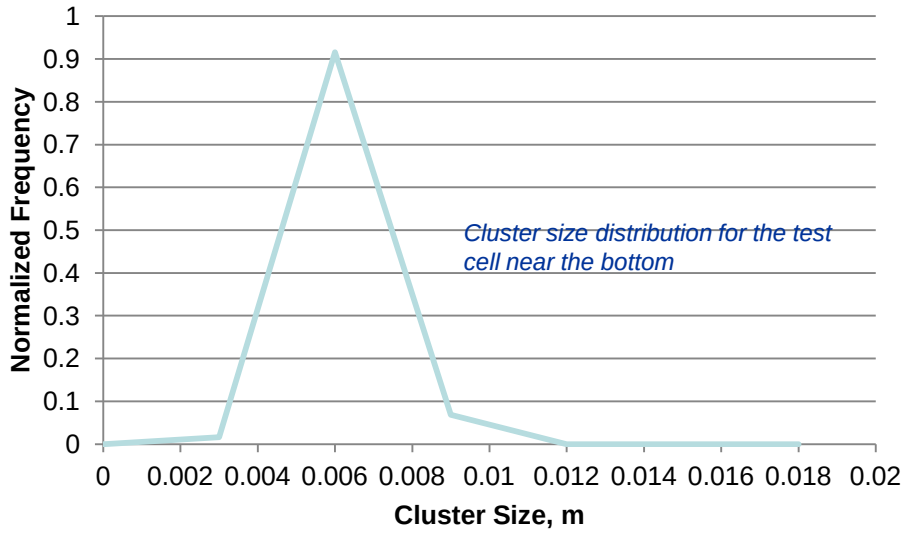
Input	Value	Units
Coal Proximate Analysis		-
Fixed Carbon	0.402	-
Volatile Mater	0.329	-
Moisture	0.223	-
Ash	0.046	
Particle Properties		
Density	2850	kg/m^3
Size	100	μm
Flow Input		
Fluidizing/Transport Air	0.00276	kg/s
Recycle solids	0.1	kg/s
Recycle gas	0.0002	kg/s
Coal	0.001	kg/s
Coal transport gas	0.0001	kg/s

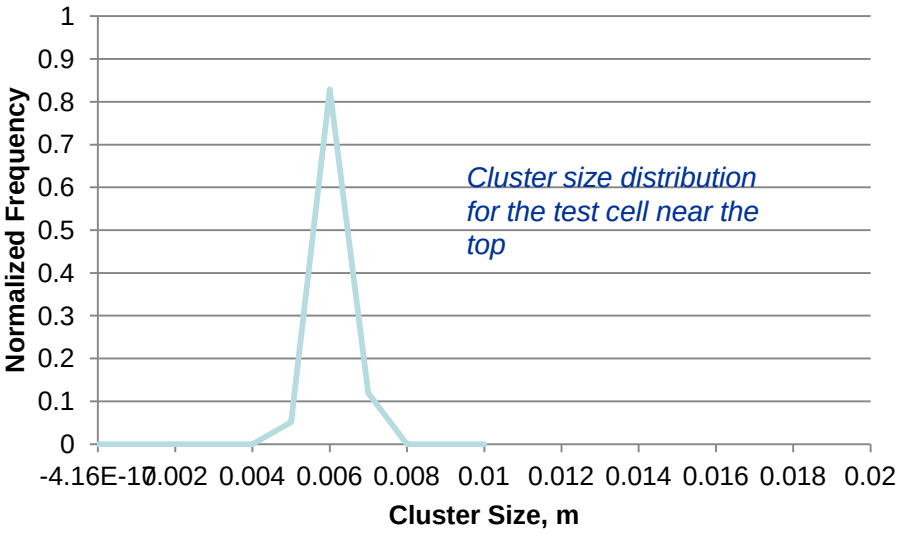
Simulation Geometry



- **The 2-D simulation was for a gasifier 0.1 m in width and 6 m in height.**
- **The grid is 10 by 600 with cells 0.01m by 0.01 m.**
- **Air at 533 K is fed through the bottom.**
- **Recycle solids and gas enter at 1117 K.**

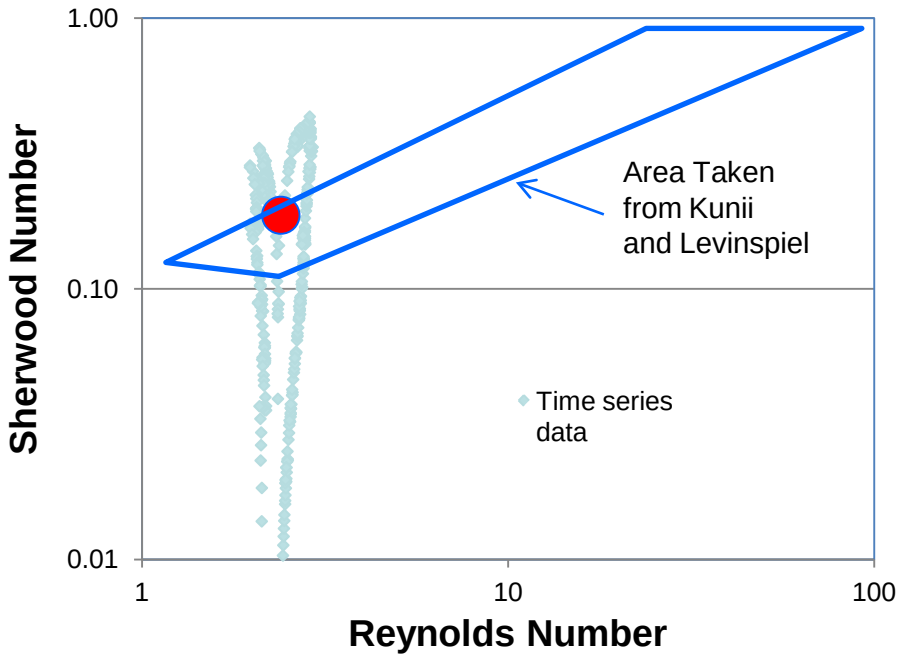
Simulation Cluster Size Distribution





- **The cluster size distribution is wider in the lower regions of the riser than the higher regions.**
- **The wide cluster size distribution at the lower cell indicates stronger non-uniformity in the solids flow as compared to that at the higher cell.**
- **The average solids fraction at the lower cell is 5.4% and 4.8% at the higher cell.**
- **The mean cluster size higher up in the riser approximately 0.0053 m and is slightly lower than that near the bottom, 0.0056 m.**

Sherwood Number from Simulation



- **The points generally arranged vertically about a Reynolds number of 3 are the values for the time series data.**
- **The large circular point is the average for the time series data.**
- **The region enclosed with the polygon reflects the data presented by Kunii and Levenspiel.**
- **There is good agreement between the simulation data and the literature data providing validation of the model predictions compared to literature data.**

Relative Effect of Mass Transfer (REMT)

The REMT is defined according to

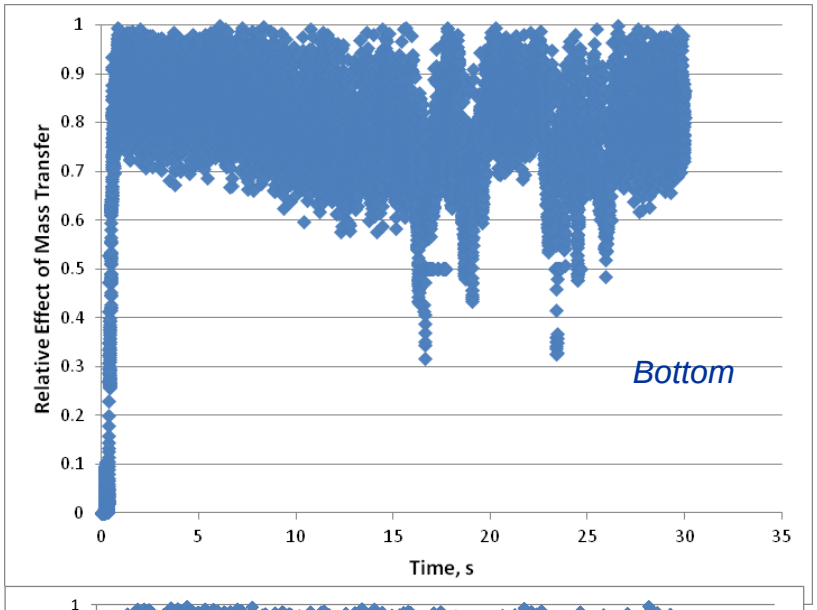
$$REMT = 1 - k/k_r$$

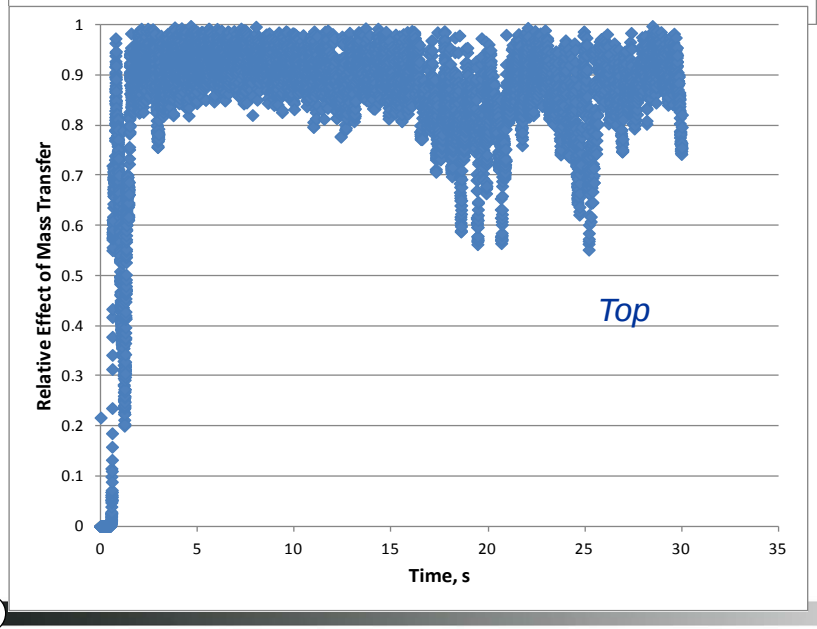
where k is found from

$$k = \frac{1}{\left(\frac{1}{k_r} + \frac{1}{k_f}\right)}$$

and k_r is the reaction rate constant for the reaction being considered.

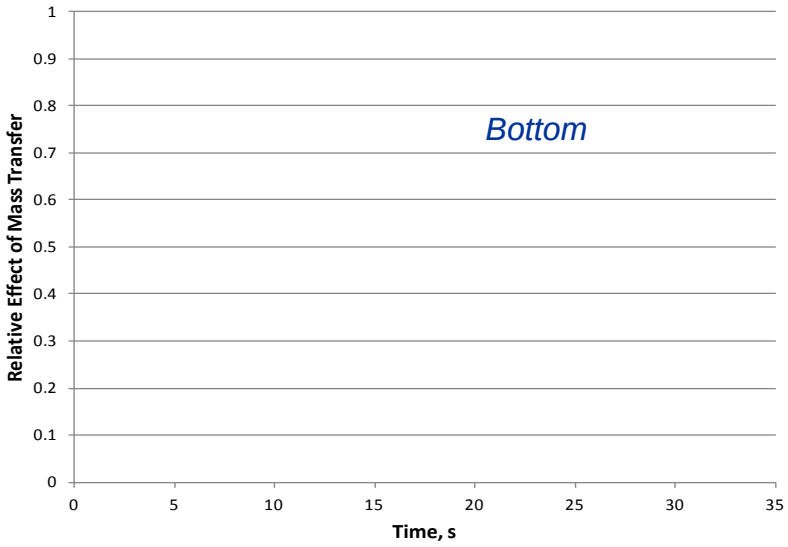
REMT for the Reaction C + .5 O_2 → CO

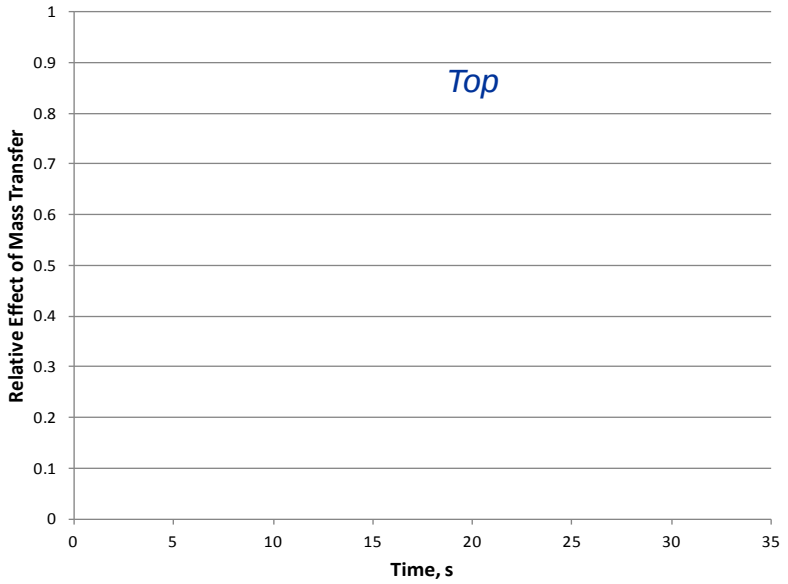




- The REMT for both of these locations is very high, indicating that mass transfer needs to be considered.
- Even though the REMT for this reaction is nominally greater than 0.6, mass transfer needs to be considered anytime the REMT is greater than about 0.05.
- Once the flow is established, the REMT for this reaction ranges between 0.3 and 1 for the cell at the bottom and 0.55 and 1 for the cell near the top.
- It can be seen that the REMT is greater for the cell with smaller clusters, lower solids fraction and slightly higher cluster fluctuating velocity.

REMT the reaction $C + H_2O \rightarrow CO + H_2$





- **Generally, similar behavior in the REMT is observed for this reaction as was observed for the $C + .5\ O_2 \rightarrow CO$ reaction.**
- **The REMT tends to range from 0.01 to 0.2 with some values as high as 0.9 for the cell near the bottom and from a value of 0.03 to 0.4 with some values as high as 0.9 for the cell near the top.**

Summary

- A new mechanistic mass transfer coefficient algorithm has been developed based upon earlier work of Breault et al and incorporated into the baseline CFD code.
- The code uses the local hydrodynamics to estimate the cluster size and fluctuating velocity in every cell to calculate the local mass transfer coefficient.
- The instantaneous values for the corresponding Sherwood number were compared with data presented in the literature with good agreement.
- The calculated values for the Sherwood number are consistent with earlier work to be an order of magnitude lower than that predicted by Gunn's correlation which has been used in the default code for the carbon – oxygen reaction only.
- The incorporation of the new mass transfer model into the baseline code gives the expected behavior for all the gasification reactions evaluated in the paper.
- At the expected and typical design values for the solids flow rate in a riser gasifier it has been shown to be significant and should be used such that the conversions are not over predicted.
- Its behaviors with changes in solids flow rate are consistent with the changes in the hydrodynamics.

Limitations and Future Work

- The cell size, at this time, is limited to have edges on the order of 1 cm.
- This limitation is made to approximate the probe size in the work of Guenther and Breault.
- Here, the functionality developed and presented for ideal 2-D clusters is generalized for 3-D clusters assuming no change in the functional form of that equation.
- It is expected that continued research will be conducted to develop a grid-independent model for the cluster size.