CFD Simulation of Fisher-Tropsch Synthesis in Slurry Bubble Column

By Andrey Troshko
Prepared by Peter Spicka

Fluent Inc.
10 Cavendish Court
Lebanon, NH,03766
www.fluent.com

Motivation & Objectives

- Internal FLUENT effort to provide guidelines and best practices for bubble column simulations with chemical reaction
- To study the effect of gas superficial velocity and slurry concentration on production rate
- 3D time dependent simulations
  - Gravity and drag are main interfacial forces acting on bubbles
- Production rate and syngas conversion was compared to 1D empirical model of C. Maretto & R. Krishna, Catalysis Today, **52**, 1999

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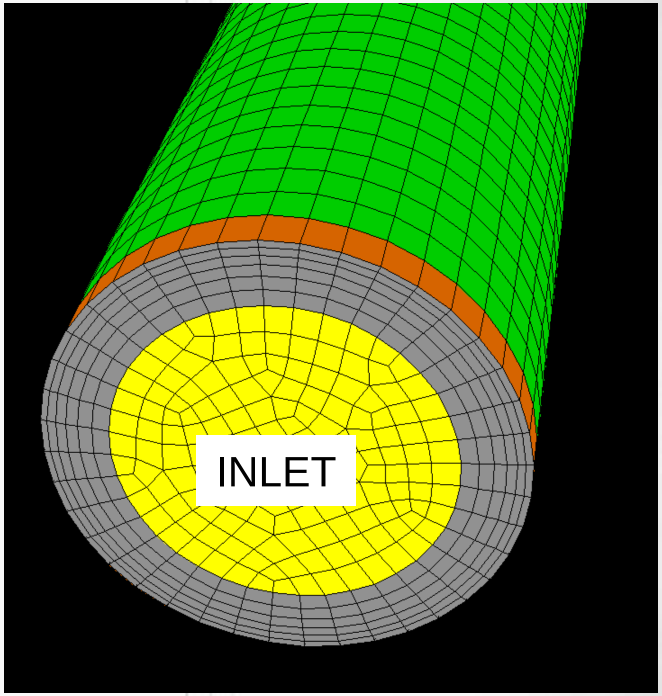
Model settings

- Euler/Euler three-phase model
- Industrial size column (H= 30 m, D= 7 m)
- Column operates in churn-turbulent regime
- Two bubble classes of 5 and 45 mm
- No coalescence/break up model assumed
- For each gas velocity two catalyst volume fractions were investigated: 20% and 35%
- Catalyst VOF defines bubble size distribution, slurry properties and CH_2 production rate
- Mesh size of ~30,000 prismatic cells



Inlet/outlet boundary zones

Inlet boundary

- Two different inlet gas velocities of 15 and 40 cm/sec
- Inlet area aerated at 50%
- Pressure at 30 bar and temperature at 240 C

Outlet boundary

- Implicit definition through degassing boundary condition with zero liquid axial velocity
- Outlet surface is velocity inlet boundary condition
- Values of all variables are defined through a UDF and extrapolated from adjacent cell center
- Gas vertical velocity is set to some value, say, 3-4 times gas superficial velocity
- Additional sources for any variable ϕ_{liq} in liquid phase are defined as:

$$S_{\phi_{liq}} = \phi_{liq}\left(\rho_{liq}\vec{U}_{liq} \cdot \vec{A}_{cell} / V_{cell}\right)$$

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Drag law and turbulence model

- Bubble size and drag law
  - If bubble diameter is 1-10 mm, then $C_d = 0.666 d_b \sqrt{g(\rho_{liq} - \rho_{gas})/\sigma}$
  - If bubble diameter is larger than 1 cm, then $C_d = 2.6666$
  - **One can also use effective single bubble size with churn turbulent regime such as it is between smallest and largest size**
- Turbulence model recommendations
  - The following is a recommended procedure for choosing turbulence model
    - Standard k-eps model overestimates energy dissipation and results in stuck gas plume
    - RNG mixture model is recommended instead
    - If plume is stuck with RNG mixture, use RNG per phase or decrease C_μ by factor of 10

Phase properties & numerical settings

- Slurry viscosity based on Einstein equation $\mu_{SL} = \mu_L (1 + 4.5\varepsilon_S)$
- Slurry density calculated as $\rho_{SL} = \rho_L \left(1 - \frac{\rho_L}{\rho_{SK}} \varepsilon_S \right) + \rho_P \varepsilon_S$
- Density of Syngas ~7 kg/m^3

Numerical parameters

- For all simulations, a time step of ~0.01 was used
- For mixed and hex meshes, high UR factors and 4 iterations per time step are recommended
- All variables should be discretized with QUICK scheme
- If solution diverges during first iterations, discretize all variables with Upwind, run for 1-2 time steps, than switch back to QUICK

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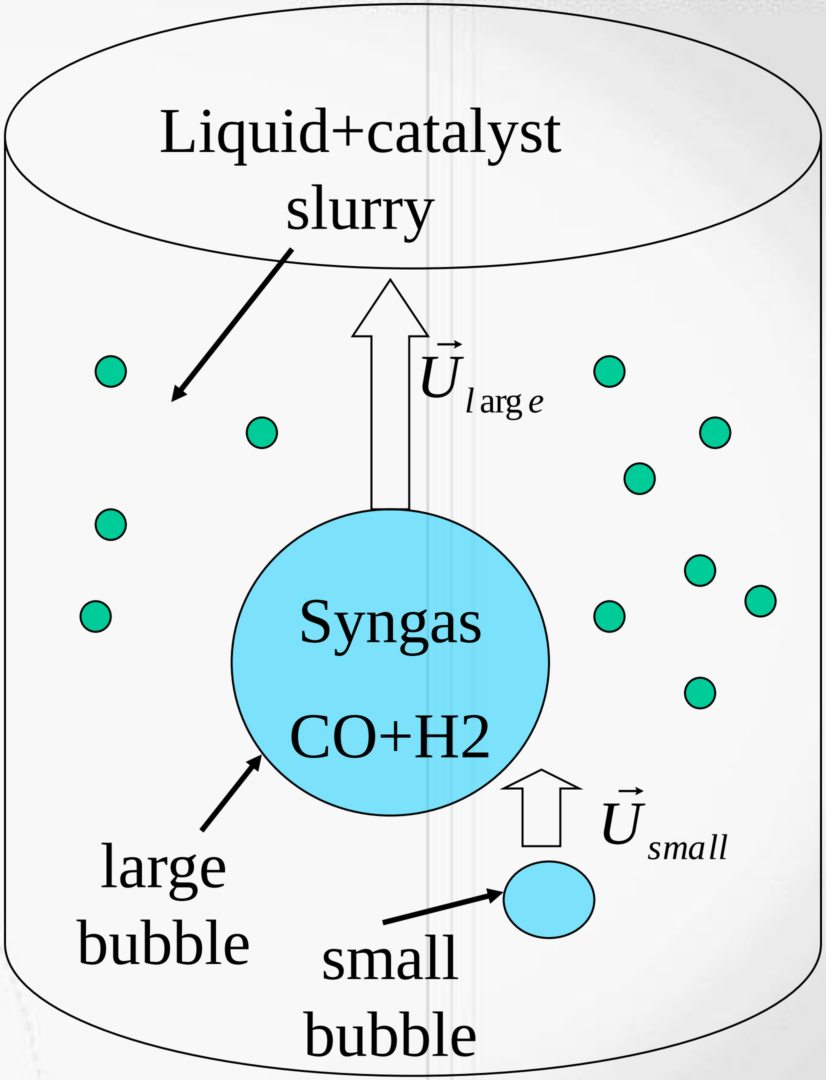
Chemical reaction

- Three phase model:
  - Small bubbles ~0.5 cm
  - Large bubbles ~4.5 cm
  - Slurry liquid
- Two stages Fischer-Tropsch synthesis
  - Heterogeneous:
    - CO_{gas}=> CO_{liq}
    - H_2O_{gas}=> H_2O_{liq}
  - Homogeneous
    - $CO_{liq}+2H_{2\ liq}$ => $CH_{2\ liq}+H_2O_{liq}$



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Reaction rates

- Homogeneous reaction rate in liquid is:
  - $CO_{liq}+2H_{2\,liq}=>CH_{2\,liq}+H_2O_{liq}$

$$\dot{R}^{hom}_{small/large} = a\alpha_{liq}c_{CO,liq}c_{H_2,liq}\left(1+bc^2_{CO,liq}\right)^{-1}\rho_{cat}\alpha_{cat}$$

Reaction constants

Density and VOF of catalyst

- Heterogeneous reaction rate for CO is:
  - $CO_{gas}=> CO_{liq}$

$$R^{het}_{small/large} = \alpha_{small/large}(k_L a)_{small/large}\left(\frac{c_{CO,small/large}}{m_{CO}} - c_{CO,liq}\right)$$

Reduction of CO concentration at gas-liquid interface

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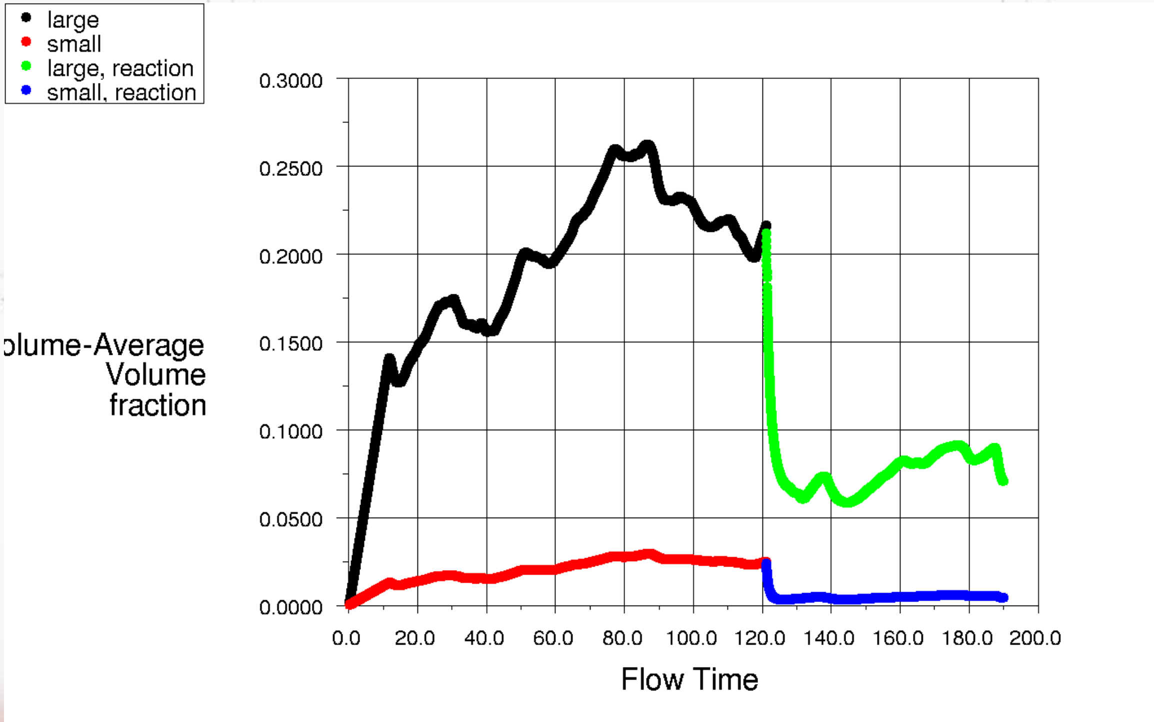
Volume fraction evolution

Time evolution of VOF before and after reaction start-up



Overall gas volume fraction

J_{gas}, cm/s	15	15	40	40
α_{cat}, %	20	35	20	35
VOF of small bubbles [%] Without reaction With reaction	0. 94 0.045	3.16 0.21	0.7 0.07	2.5 0.46
Overall gas holdup [%] Without reaction With reaction	13 1.3	14 1.0	24 7.9	24 4.7

Catalyst volume fraction strongly affects small bubble volume fraction but not overall holdup

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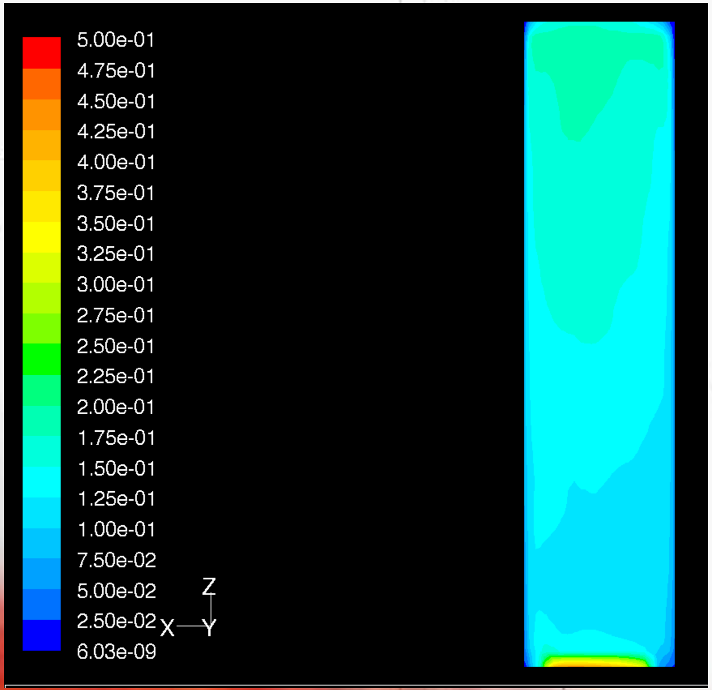
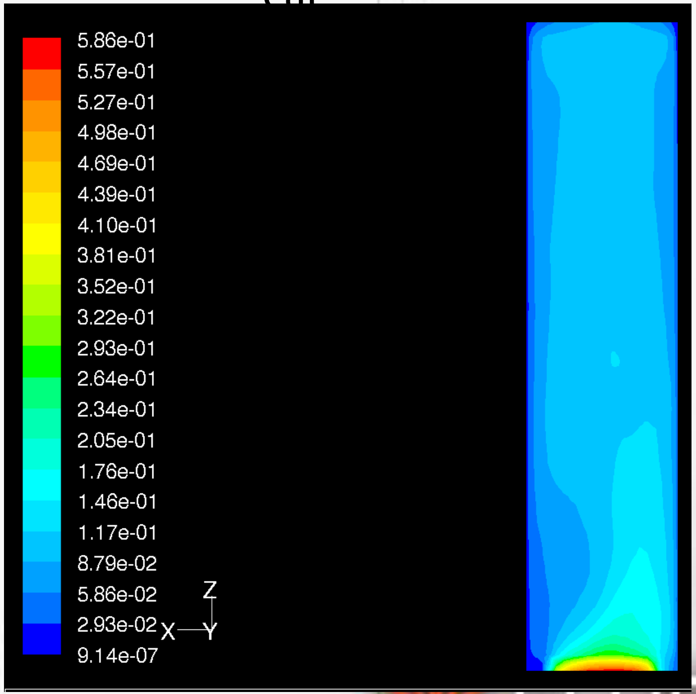
VOF of large bubbles

- Results for J_{gas}=40 cm/sec, α_{cat}=20% and α_{cat}=35%

α_{cat}=20%



α_{cat}=35%



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VOF of small bubbles

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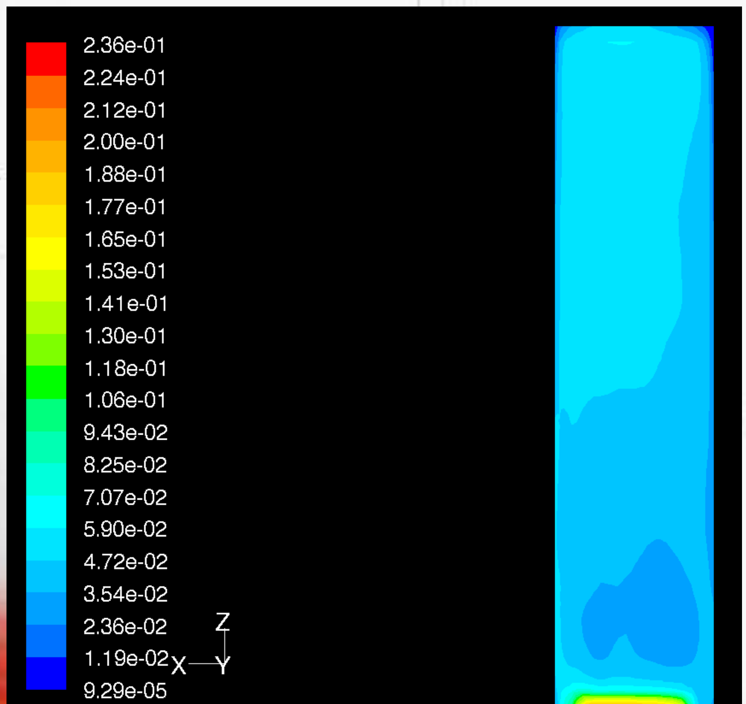
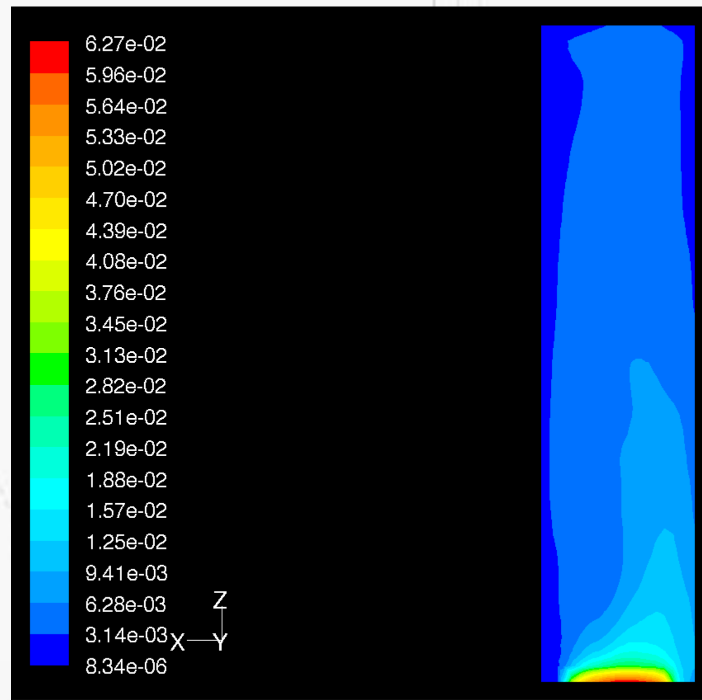


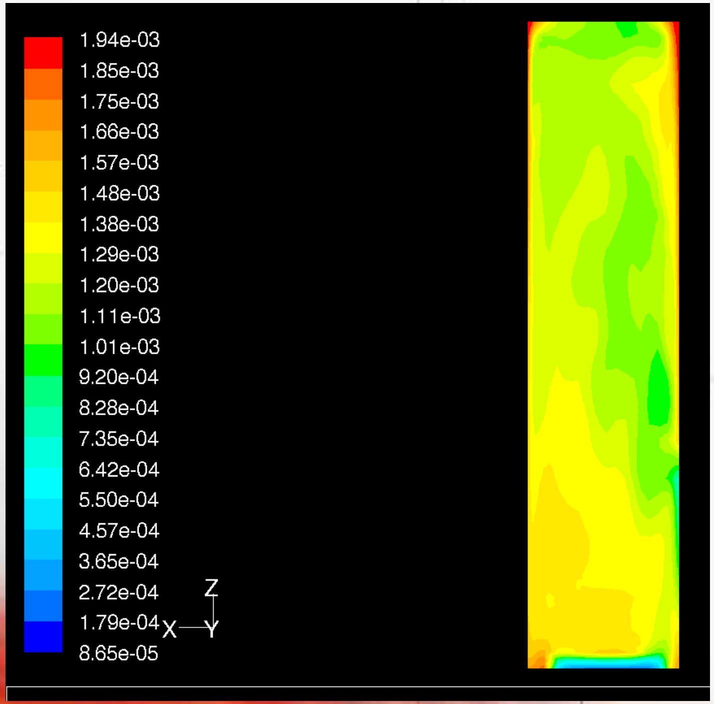
α_{cat}=35%



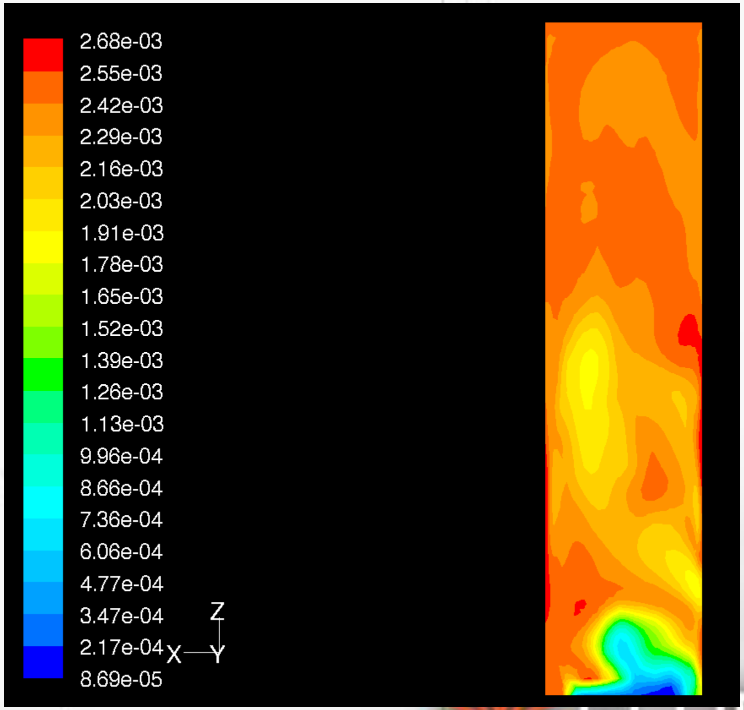
Homogeneous reaction rates

- Results for J_{gas}=40 cm/sec, α_{cat}=20% and α_{cat}=35%

α_{cat}=20%



α_{cat}=35%



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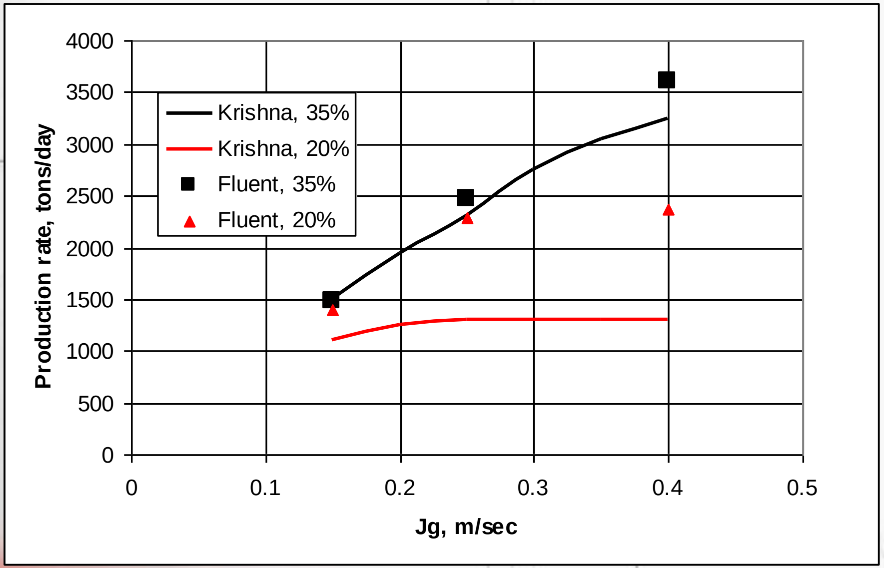
Comparison of production rate of CH_2

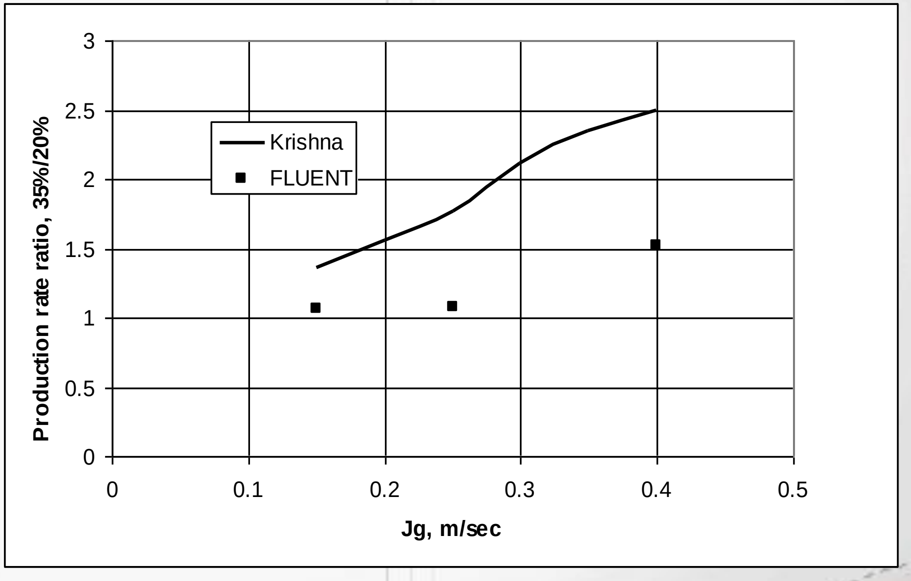
Time averaged values

α_{cat}=20% and 35%



Influence of catalyst concentration on production rate

p. rate(α_{cat}=35%)/ p. rate(α_{cat}=20%)



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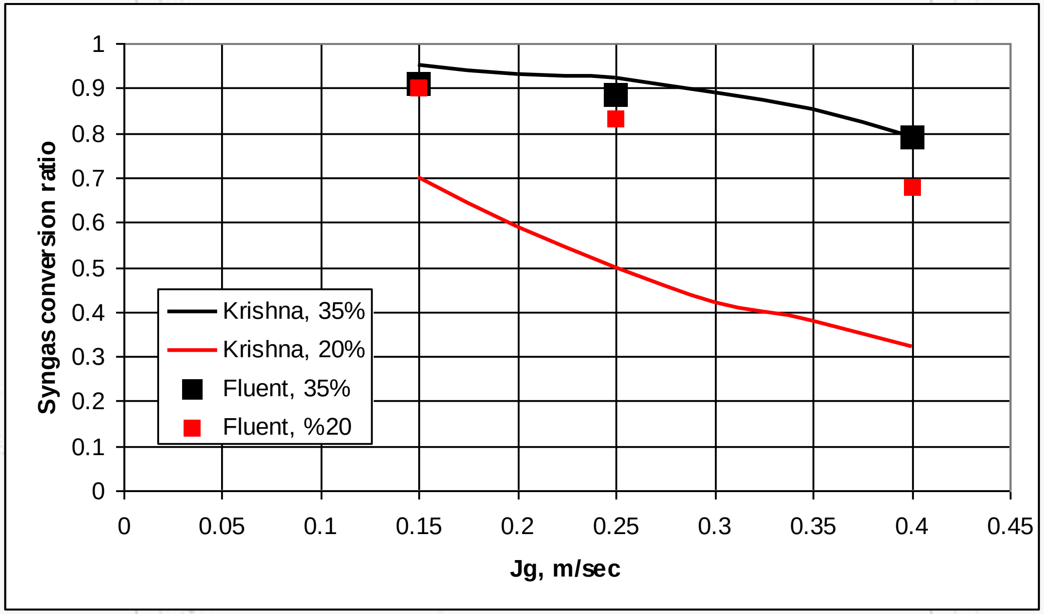
Syngas conversion ratio comparison



- At lower gas flow rate, conversion is almost independent of slurry concentration
- Conversion decreases with gas flow rate

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Conclusion

- Bubble column simulation should be 3D and time dependent to capture essential dynamics
- Turbulence model is essential to capture bubble plume movement
- RNG k-eps per phase or mixture appears to ensure plume dancing, but it is very far from clear whether they predict turbulence field in liquid correctly
- Two bubble size model with realistic chemistry appears to adequately predict main trends in real production size bubble column
- Additional improvement can include bubble-bubble interaction with population balance