Solar pyrolysis of methane

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Abstract

- Currently, 50% of H_2 is produced via steam methane reforming process (SMR), which is not environmentally-friendly.
- Methane pyrolysis can compete favourably with SMR.
- Methane pyrolysis in a liquid bubble column (Figure 1a) offers potential to mitigate the challenges of using solid catalyst such as cocking. It also offers method for in-situ separation of product carbon.
- Methane pyrolysis in a molten catalyst is a new technology.

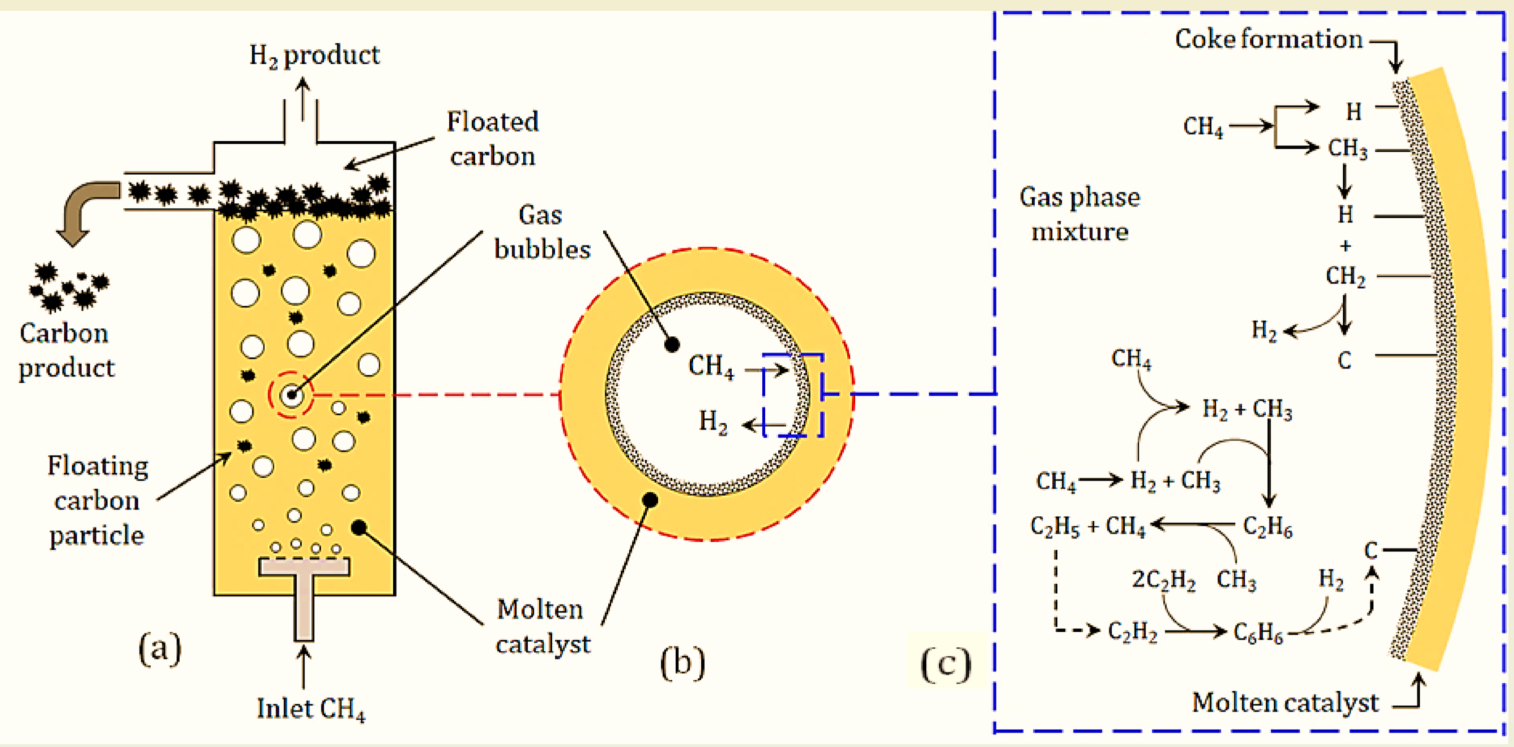


Figure 1: Schematic representation of a) A bubble column reactor for methane pyrolysis, b) Single reacting bubble, c) Methane pyrolysis reaction on the surface of the methane bubble.

There is a need for developing a fundamental understanding on the mechanism of methane pyrolysis within a bubble (Figures 1a-c). The overall objective of this project is to meet this need.

Methodology

- There are some models in the literature on the methane pyrolysis within a bubble [1-3]; however, they are based on several simplifying assumptions. Present calculations show that the bubble radius and terminal velocity vary significantly while rising in the column of the liquid tin (Figure 2).

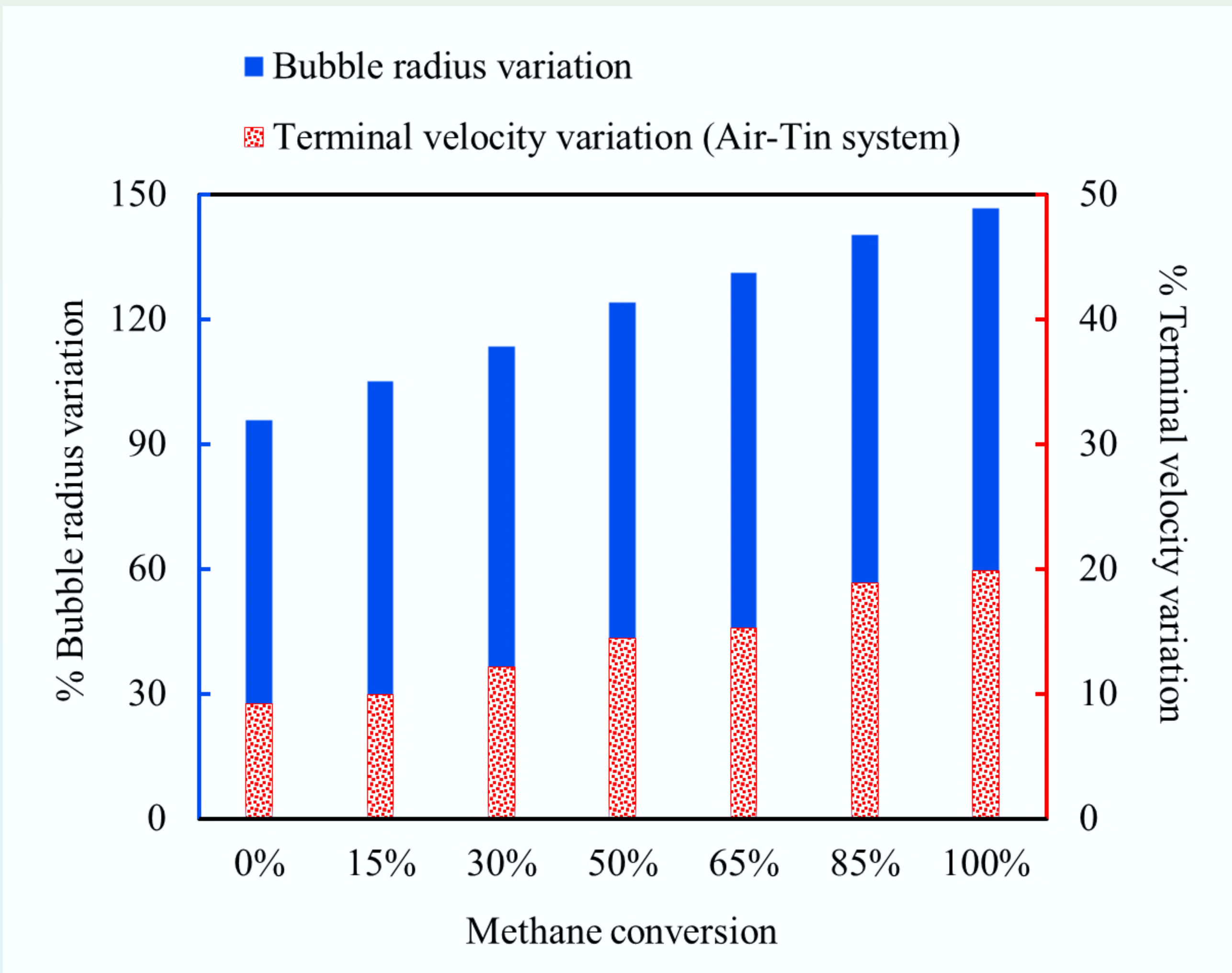
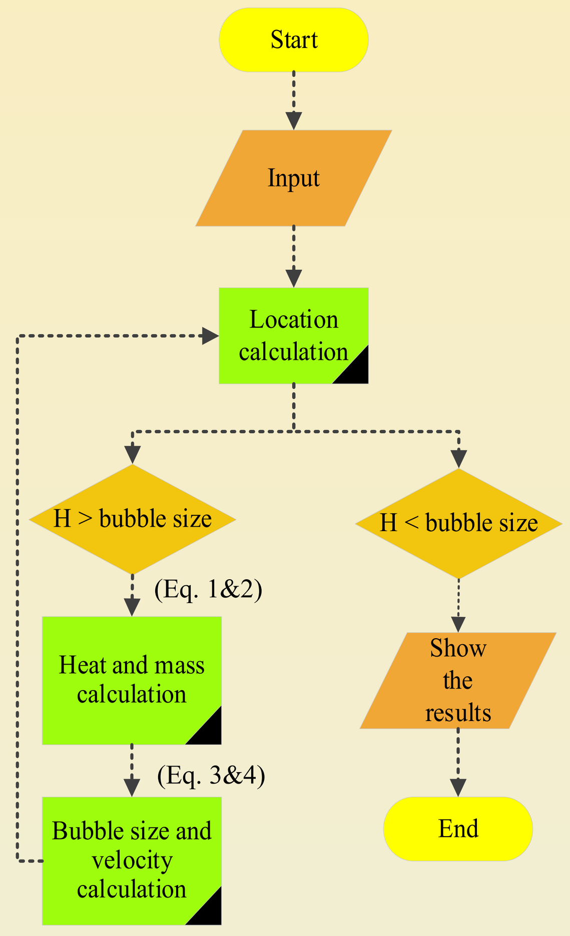


Figure 2: Bubble radius and bubble terminal velocity variations through the column of liquid tin at 0-100% methane conversion.

- Methane pyrolysis ($CH_4 \rightarrow C(s) + 2H_2 \quad \Delta H = 74.9\,\frac{kJ}{mol}$) within a rising bubble will be modelled via in-house developed codes in MATLAB (Figure 3), by simultaneously solving energy (Eq.1), mass (Eq.2) and momentum equations, to advance fundamental understanding of the process.
- Each step of the study will be validated/verified separately, due to the lack of experimental data over all operational conditions.
- The model will be used to perform a comprehensive sensitivity analysis.



$$-\frac{1}{r^2}\frac{d}{dr}\left(k\,r^2\frac{\partial T}{\partial r}\right) - \dot{Q}_{rxn} = \rho c_p\frac{\partial T}{\partial t} \qquad (1)$$

$$\frac{\partial c}{\partial t} + V_r\frac{\partial c}{\partial r} = D\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial c}{\partial r}\right)\right] \qquad (2)$$

$$V = \frac{nZR_gT}{P} \qquad (3)$$

$$U = \frac{{d_b}^2\rho g}{18\mu_l}\left(1 + \frac{Ar/96}{(1+0.079Ar^{0.794})^{0.755}}\right)^{-1} \qquad (4)$$

Figure 3: Flowchart of the code main body and equations for numerical modelling of methane pyrolysis in a bubble at a liquid tin column.

Results

- Numerical modelling is in progress. To date, the equations related to the bubble rising velocity and size variations have been solved and validated against available experimental data in the literature (Figure 4).
- In future, heat and mass transfer equations will be solve and implemented in the code.

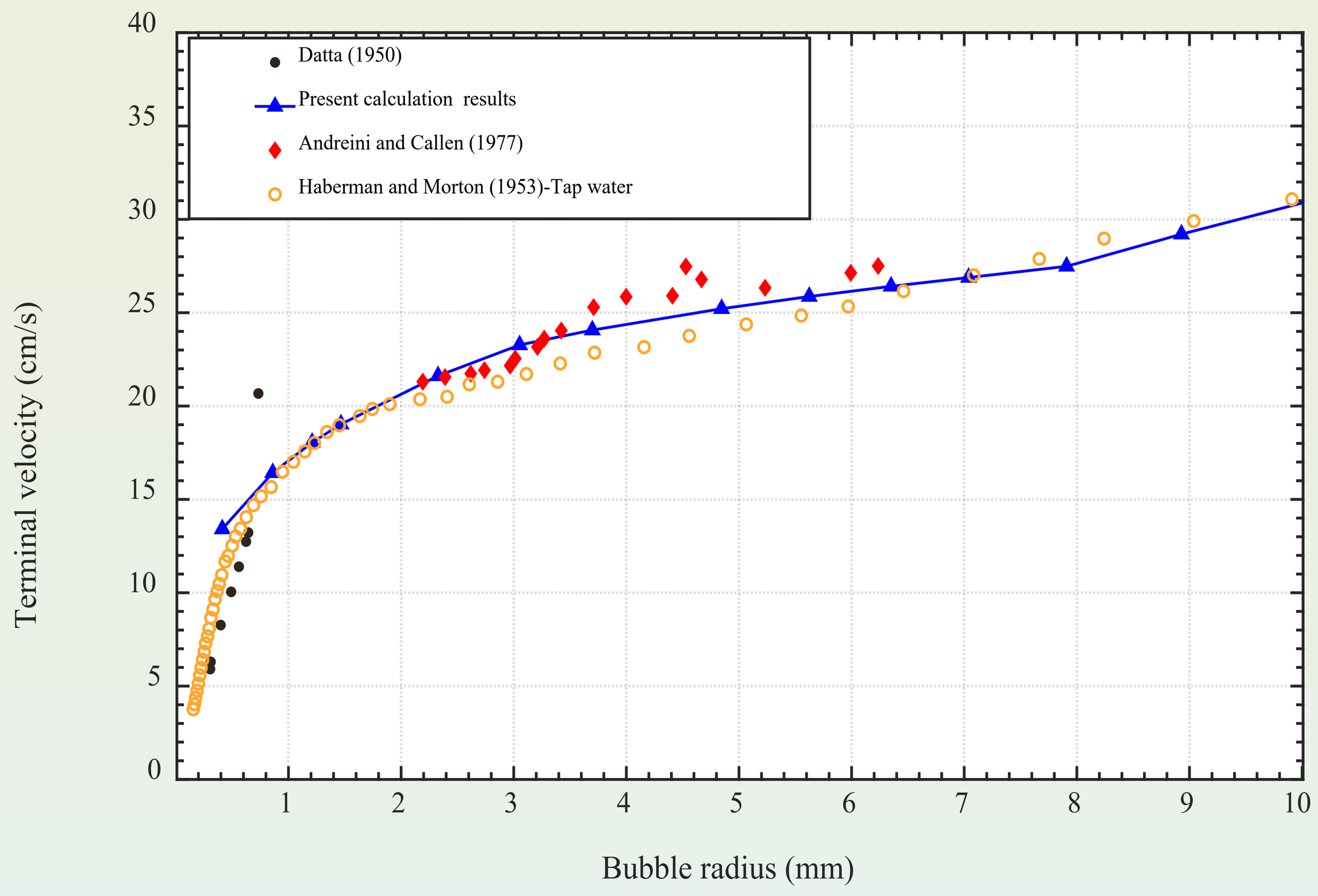


Figure 4: Comparison between the present calculated data and the experimental results in the literature.

Conclusions

- There are some models on the methane pyrolysis within a bubble at liquid metal columns, but stablished models are based on several unjustified assumptions.
- There is a need for a more accurate model.
- The developed code for the bubble size and rise velocity estimation in the liquid column is in well agreement with the experimental data available in the literature.

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