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Computational Fluid Dynamics for Microreactors Used in Catalytic Oxidation of Propane

by

Sunday Odiba

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Introduction

- **Aim:**

  Develop a versatile a suitable model for microreactor using COMSOL

- **Objective:**

  Investigate with CFD the cold flow behaviour ;

  Investigate flow and reaction analysis;

  Optimize the reactor geometry and operation conditions;

  Build the experimental reactor;

  Run experiments;

  Compare the results with the COMSOL ones.

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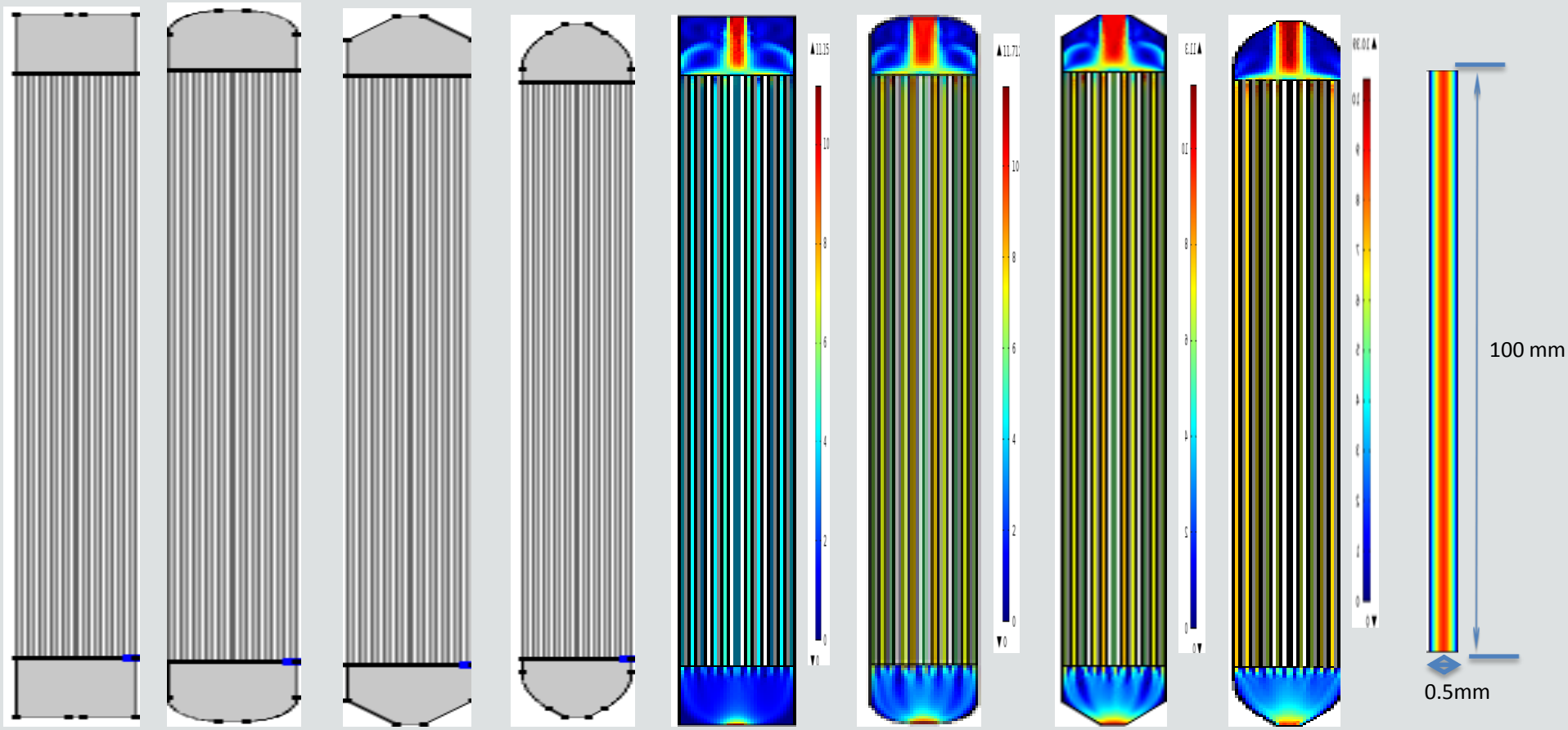
Manifold geometry



Type A1 Type A2 Type A3 Type A4 Type A1 Type A2 Type A3 Type A4

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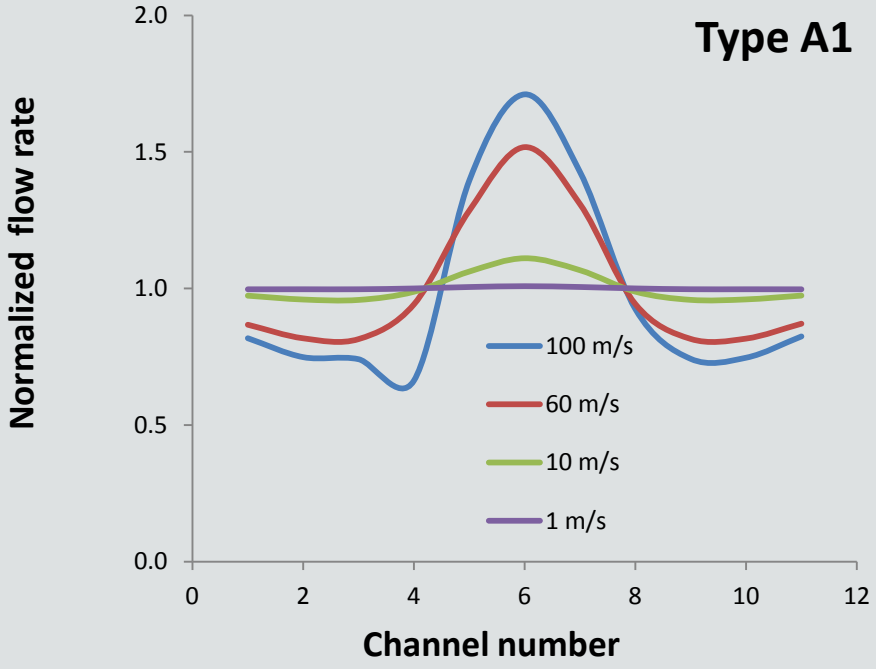
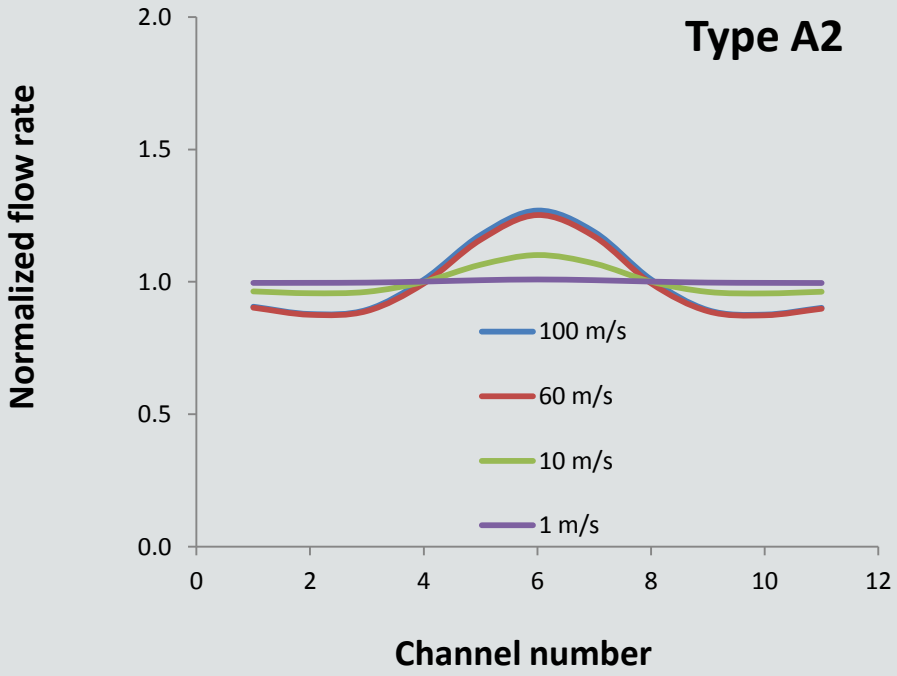
Results & discussion

Effect of inlet velocity on flow distribution within the microchannel





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Results & discussion

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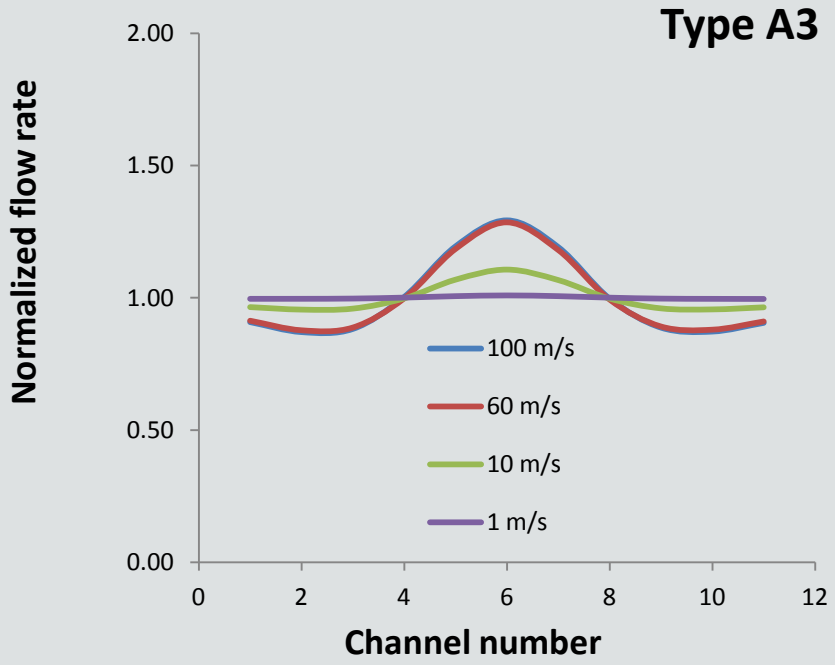

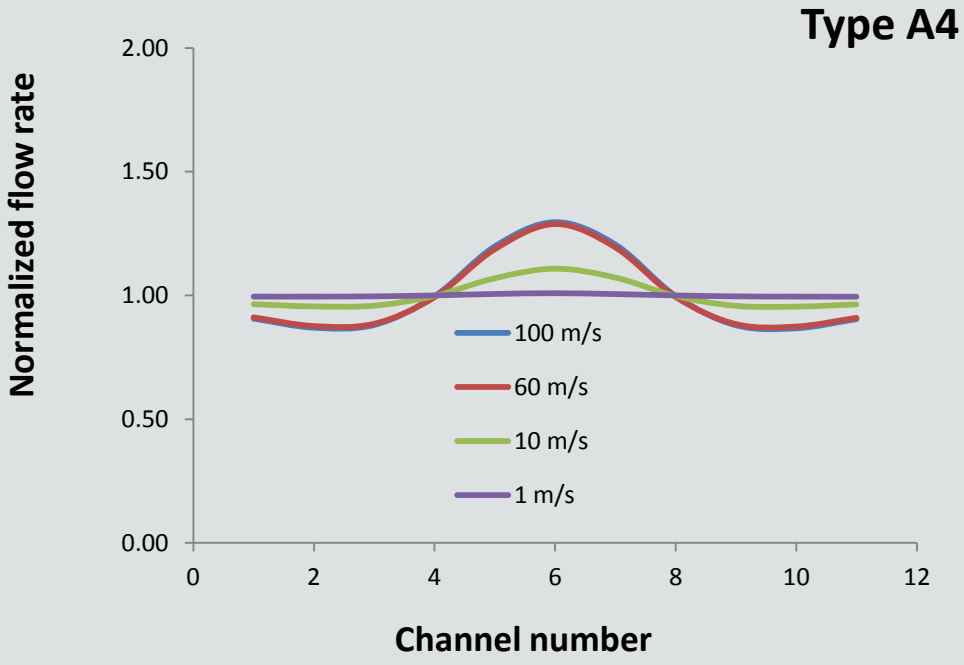

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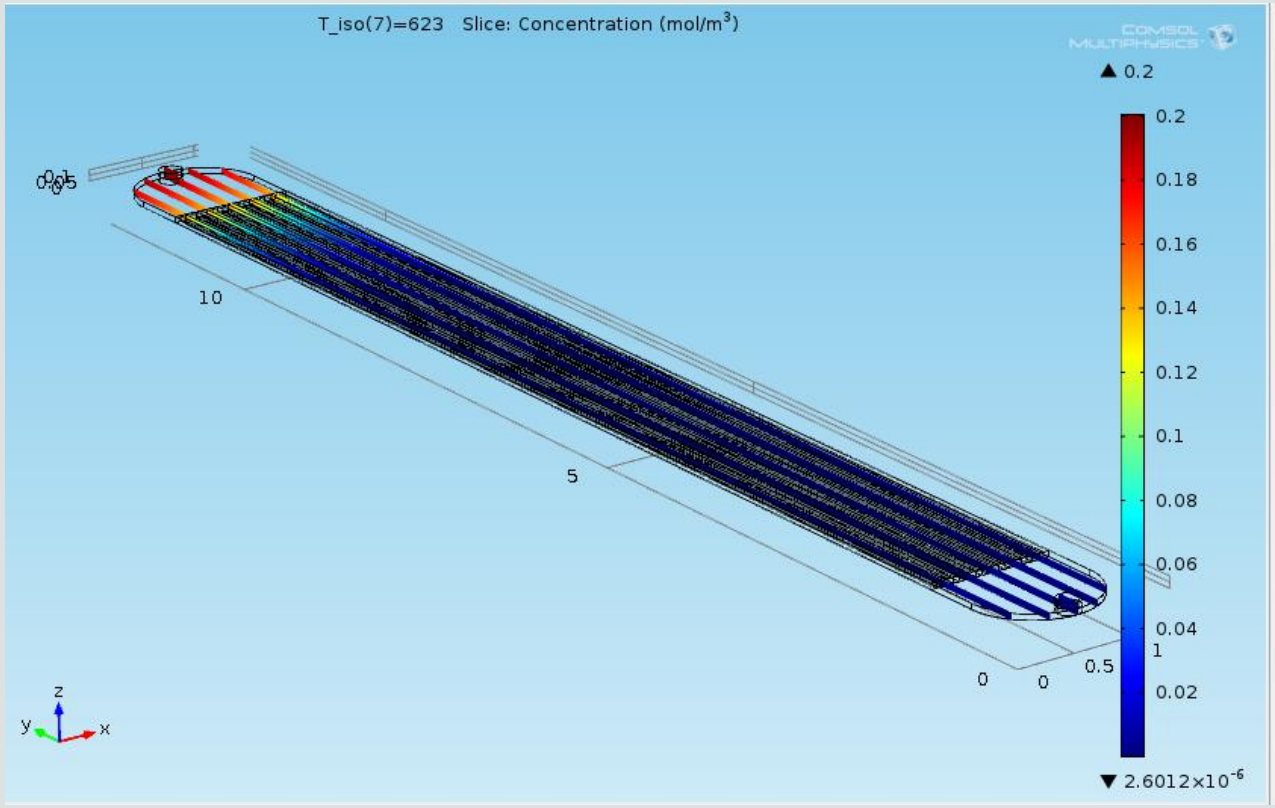
Results & discussion

Concentration gradient of propane over Au/Cr/γ-Al2O3 at inlet velocity of 0.01 m/s



$$C_3H_8 + 5O_2 => 3CO_2 + 4H_2O$$

$$r_{C_3H_8} = \frac{k_{O_2} k_{C_3H_8} P_{C_3H_8} P_{O_2}}{k_{O_2} P_{O_2} + 5 k_{C_3H_8} P_{C_3H_8}}$$

$$k_{O_2} = 1.36 \times 10^{12} \exp\left(\frac{-18125}{T}\right)$$

$$k_{C_3H_8} = 1.16 \times 10^{10} \exp\left(\frac{-15104}{T}\right)$$

(Lin, Jiunn-Nan and Ben-Zu, Wan, 2004)

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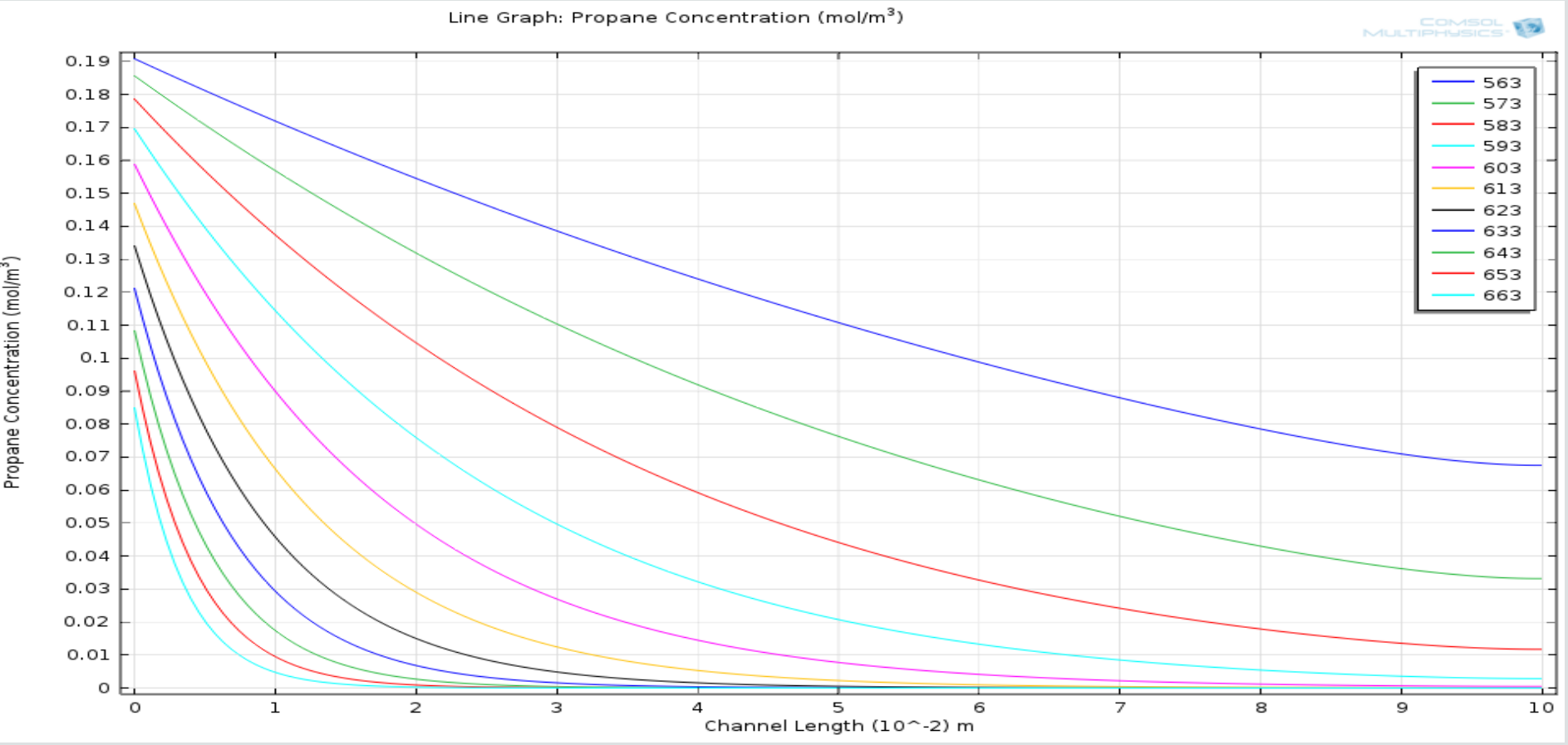
Results & discussion

Propane concentration gradient along a channel at a velocity of 0.01m/s



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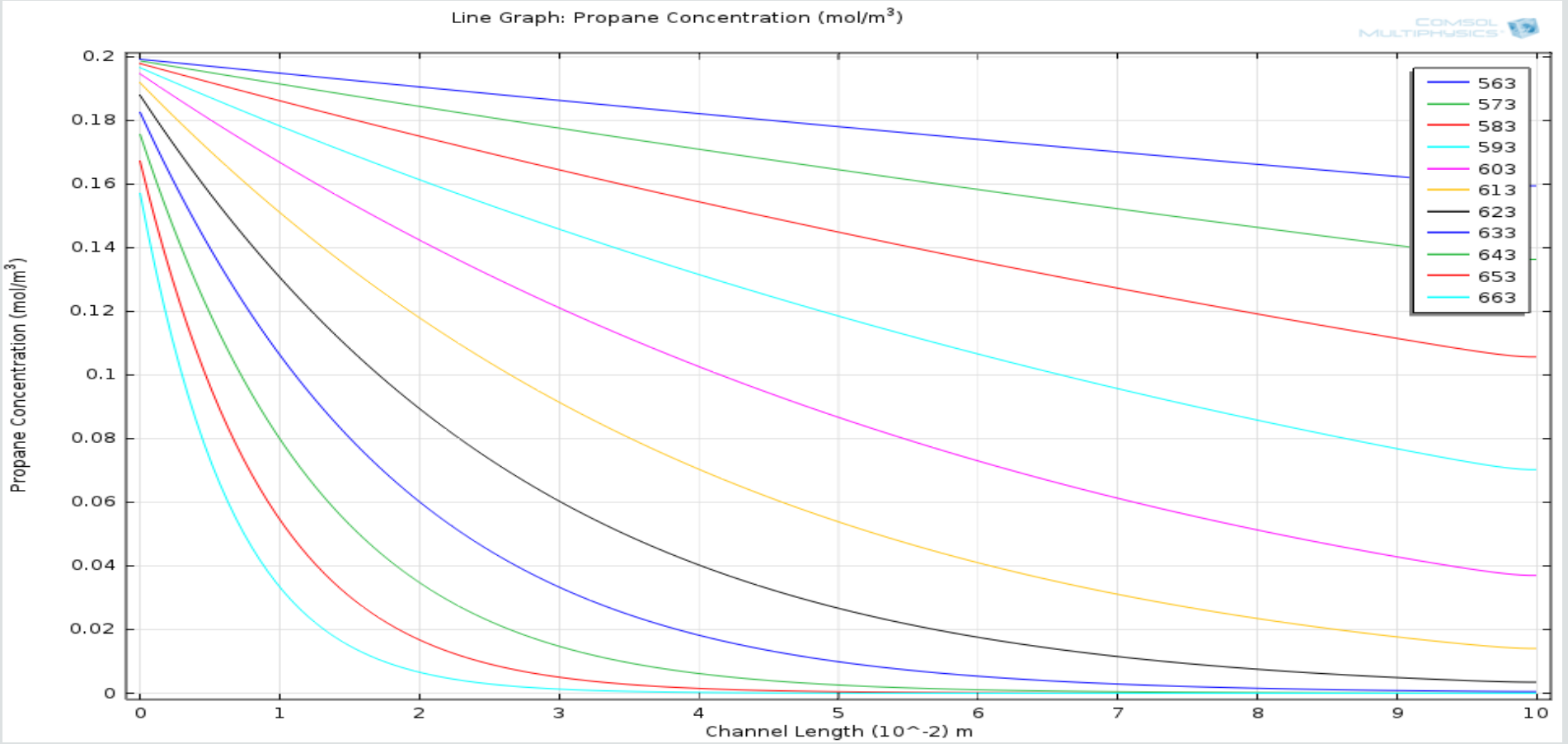
Results & discussion

Propane concentration gradient along a channel at a velocity of 0.05m/s



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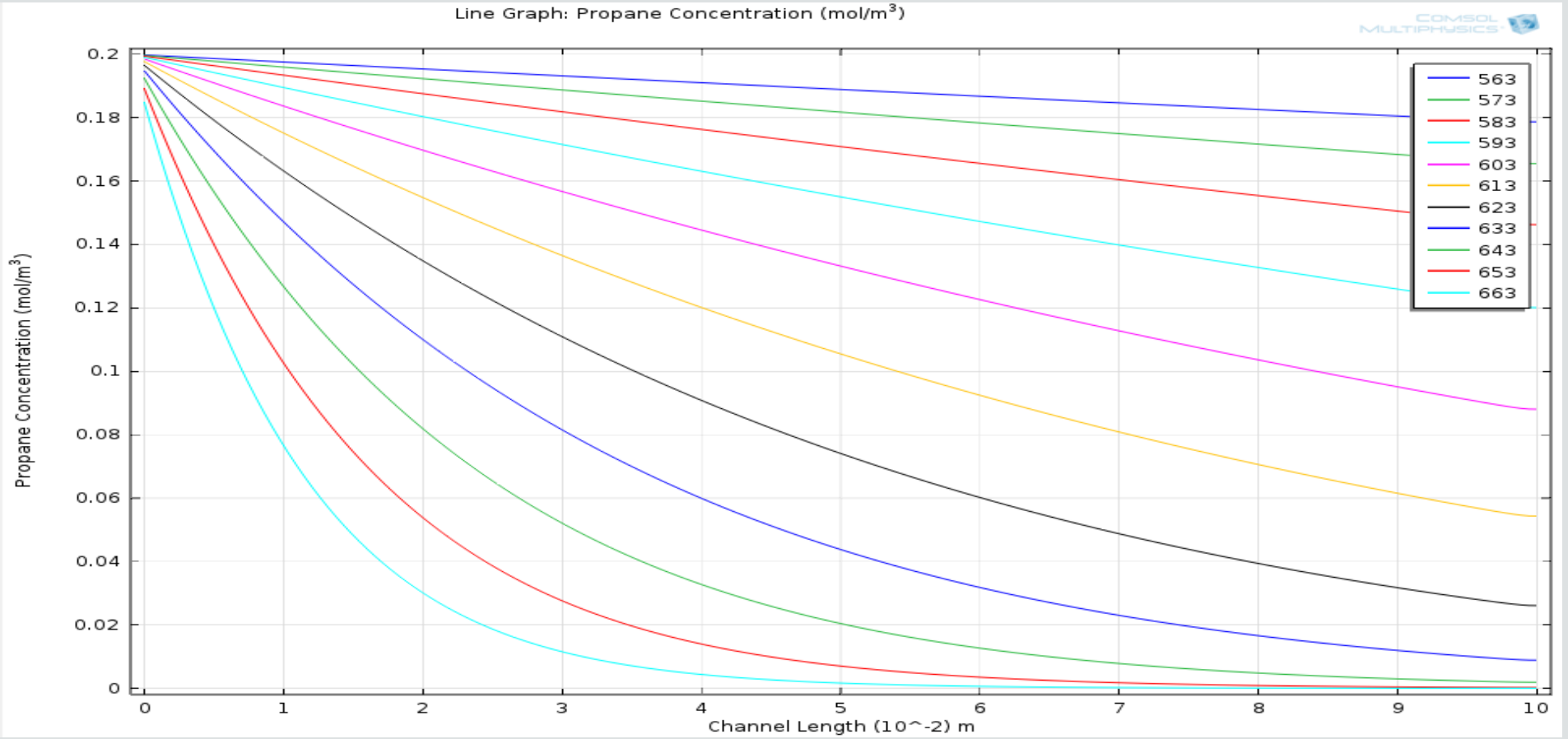
Results & discussion

Propane concentration gradient along a channel at a velocity of 0.1m/s



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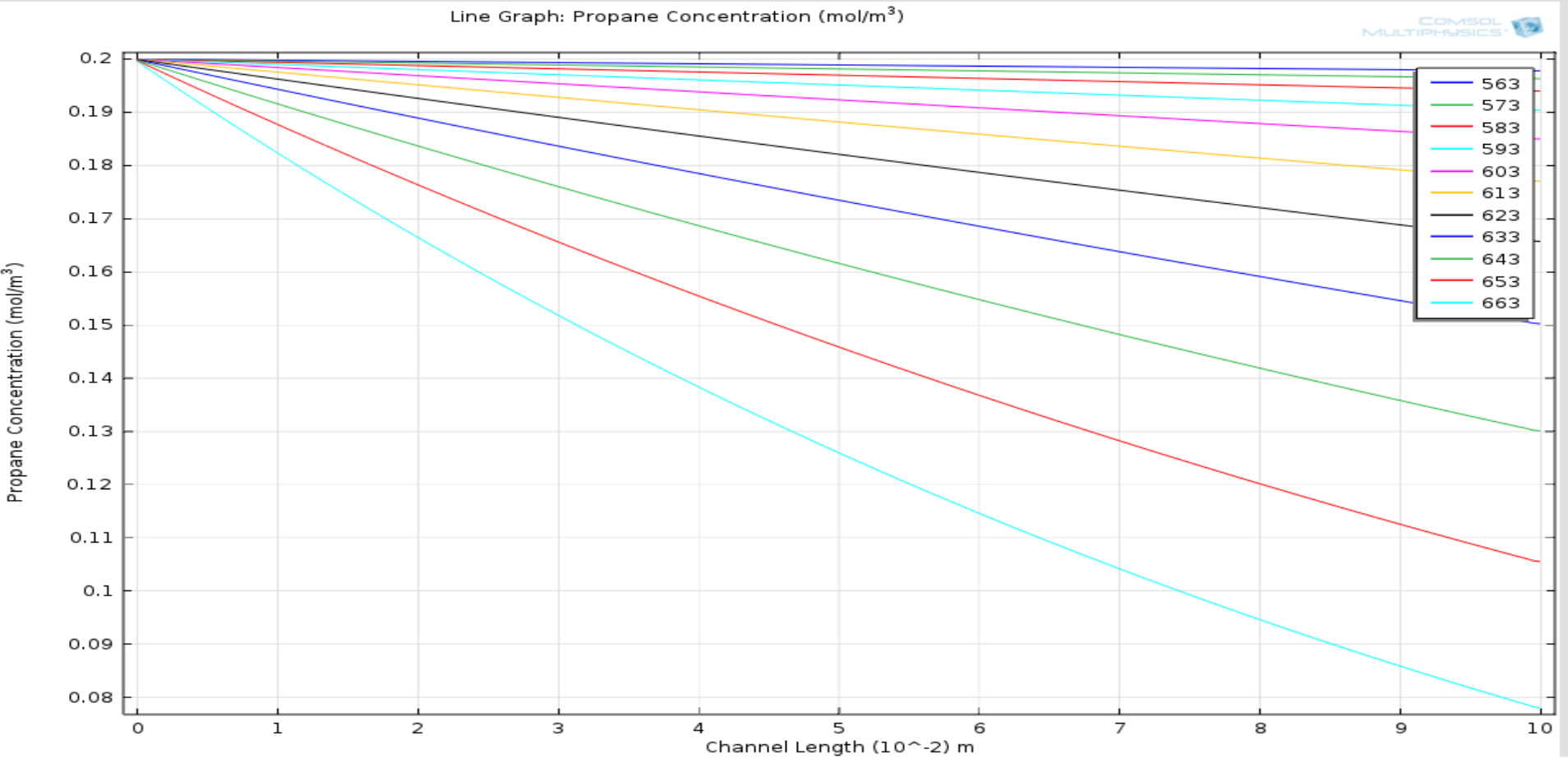
Results & discussion

Propane concentration gradient along a channel at a velocity of 1m/s



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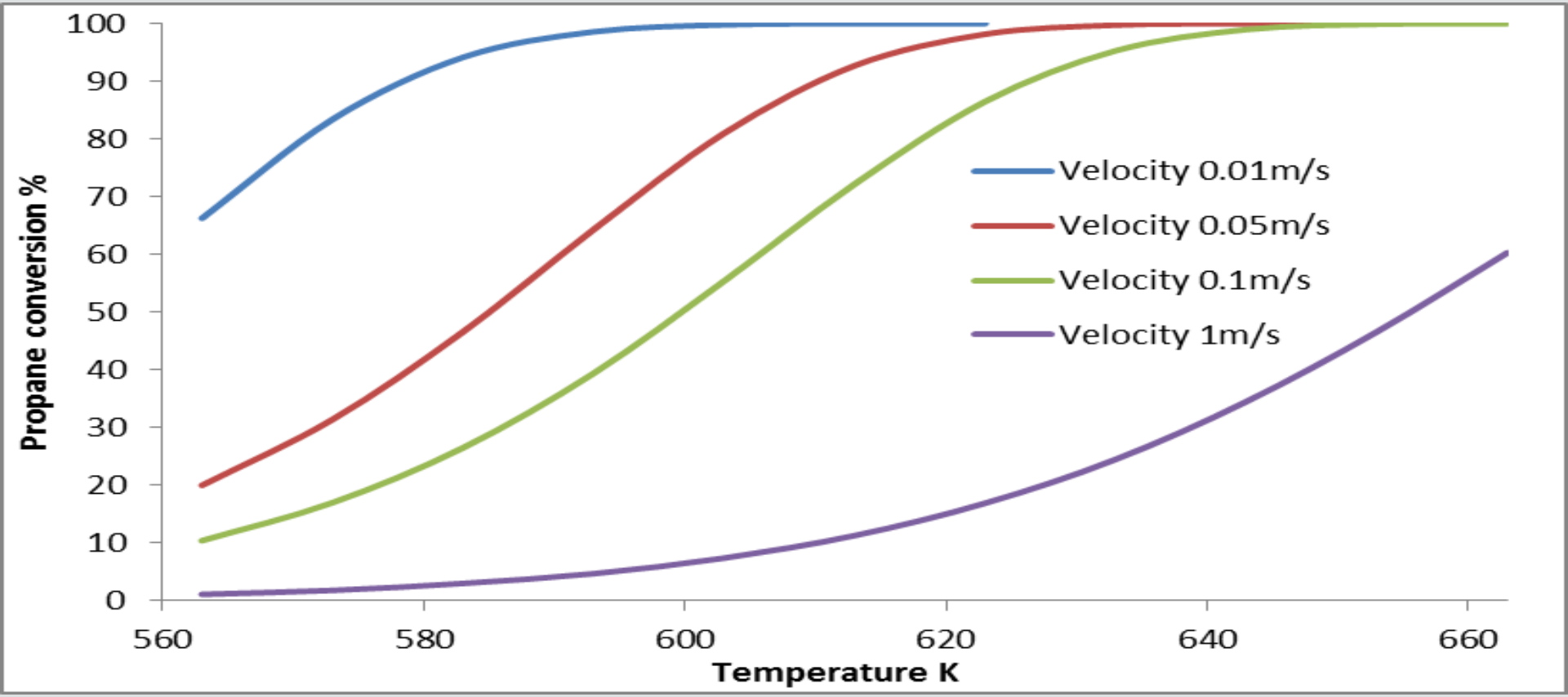
Results & discussion

Propane exit conversion against temperature at velocity of 0.01, 0.05, 0.1, and 1 m/s



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Conclusions

- ✓ Four microreactor geometries investigated;
- ✓ Flow distribution assessed based on Relative Standard Deviation;
- ✓ Type A2 gives the best flow distribution; flow behaviour from laminar to transitional;
- ✓ The simulated results have revealed that higher conversion rates of propane can be achieved by decreasing inlet gas velocity from 1 m/s to 0.01 m/s and increasing temperature from 593 K to 663 K.

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Further work

- Build the experimental reactor;
- Carry out experiments using propane oxidation on Au/Cr/γ-Al_2O_3 and compare with the COMSOL simulated results to validate the model.

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