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Numerical Study of Thermophoresis Mass Transport in Binary Fluid Mixtures Using OpenFoam

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INTRODUCTION

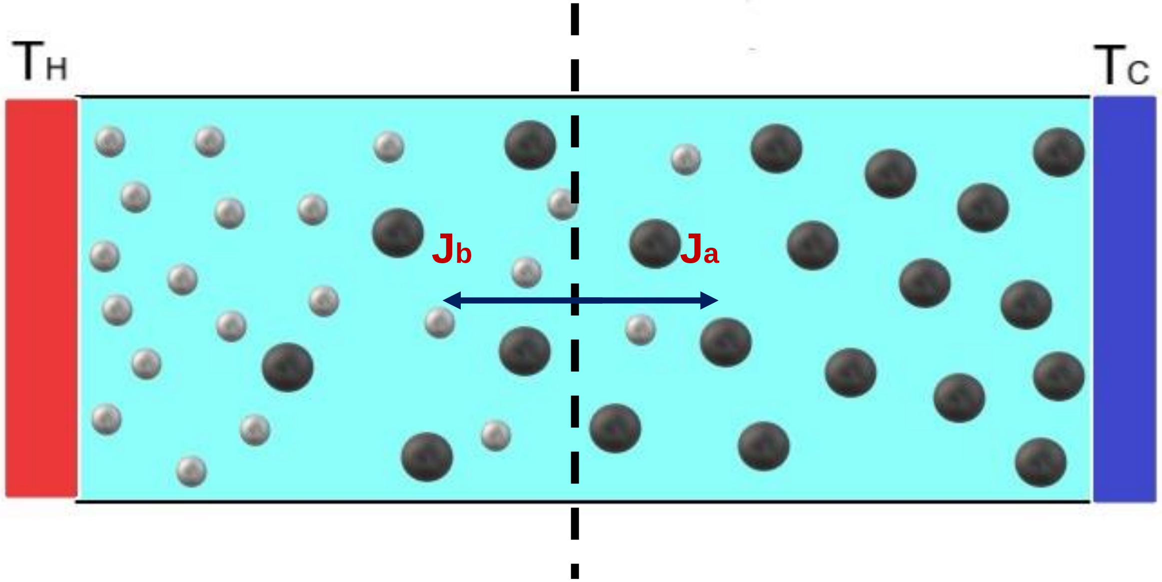
- In **fluid homogeneous mixtures**, the mass transport process induced by the dependance of species concentration on temperature gradients is known as **thermophoresis**, **thermodiffusion** or “***Soret effect***”.
- In absence of other external forces, the mass flux of the reference component “a” can be written as follows:

$$J_a = \rho D_{a,b} \nabla w_a - \rho D_T \, w_{a_0}(1 - w_{a_0}) \nabla T$$

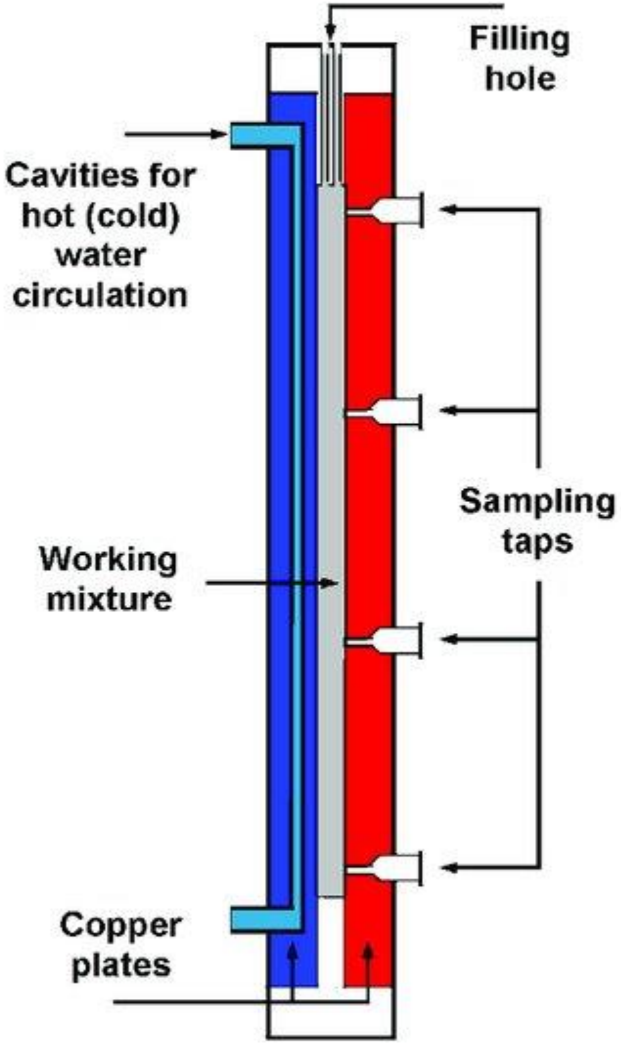
$*$ $\boldsymbol{D_{a,b}}$ is the mass diffusivity, $\boldsymbol{w_{a_0}}$ is the initial mass fraction of component “a” and $\boldsymbol{D_T}$ is the thermodiffusion coefficient.

- **For binary gaseous mixtures**: Heavy component usually moves to the colder region, while light component moves to the hotter region.
- When steady state is reached, $J_a = 0$ and concentration gradient can be written as:

$$\nabla w_a = \frac{D_T}{D_{a,b}}\ w_{a_0}(1 - w_{a_0})\nabla T$$



- Thermodiffusion transport can be found in:
  - Natural processes:
    - ➢ Thermohaline convection currents in oceans caused by the dependance of salinity gradients on temperature differences.
    - ➢ Thermo-gravitational segregation in natural hydrocarbon reservoirs.
    - ➢ Particle deposition on hot/cold surfaces, etc.
  - Industrial processes:
    - ➢ Isotope separation of liquid and gaseous mixtures with the Clusius-Dickel Column.
    - ➢ Separation and characterization of polymers.
    - ➢ Surface coating.
    - ➢ Particle decontamination.



-Sketch of a Clusius-Dickel column, Retrieved from Lapeyra et al. 2017

*Lapeyra, E., Ghebardt M., Triller, T., Mialdun, A., Kolher, W., Shevtsova, V., Mounir-Bou Ali, *M. Transport properties of the binary mixtures of the three organic liquids toluene, methanol, and cyclohexane*. 2017. The Journal of Chemical Physics. 146(9):094507.

Numerical Analysis Of Thermophoresis

- Application of CFD on thermodiffusion processes:
  - Compliments experimental analysis where visualization is **limited**.
  - Quantification and parametrization of **mass transfer dependency** on thermophysical and geometrical variables.
  - Testing of **different physical conditions** (e.g., residual or zero gravity, ideal adiabatic systems, etc.) that are hard to replicate in experimental environments.

Thermodiffusion Model in OpenFOAM

- A basic thermodiffusion model is included into OpenFOAM's ***thermophysica*l properties library**.
- Thermodiffusion coefficient is calculated with initial parameters: mass diffusivity $D_{a,b}$, initial molar fraction $x_{a,0}$, and **thermodiffusion factor $\boldsymbol{\alpha_T}$**.
- Then, thermodiffusion coefficient is corrected with the temperature variation of the simulation:

$$D_T = \frac{\alpha_T x_{a,0}\left(1 - x_{a,0}\right) D_{a,b}}{T}$$

- This new implementation was added into two solvers for **convective** and **non-convective** thermodiffusion cases.
- Laplacian solver for non-convective simulation
  - Species transport equation:

$$\frac{\partial w_a}{\partial t} += D_{a,b}\nabla^2 w_a + D_T w_{a,0}\left(1 - w_{a,0}\right)\nabla^2 T$$

  - Energy equation:

$$\frac{\partial T}{\partial t} = \alpha \nabla^2 T$$

- Compressible solver for convective simulation,
  - Navier-Stokes equation:

$$\frac{\partial(\rho v)}{\partial t} + v \cdot \nabla(\rho v) = \nabla P - \nabla \cdot \tau$$

$$\tau = -\mu(\nabla v + (\nabla v)^T) + \frac{2}{3}(\nabla \cdot v)\delta$$

  - Energy equation in terms of enthalpy:

$$\frac{\partial(\rho h)}{\partial t} + \nabla \cdot (\rho v h) + \frac{\partial(\rho K)}{\partial t} + \nabla \cdot (\rho v K) - \frac{\partial P}{\partial t} = -\nabla \cdot q + \nabla \cdot (\tau \cdot v)$$

$$q = -\kappa \nabla T; \qquad K = \frac{|v|^2}{2}$$

  - species transport equation:

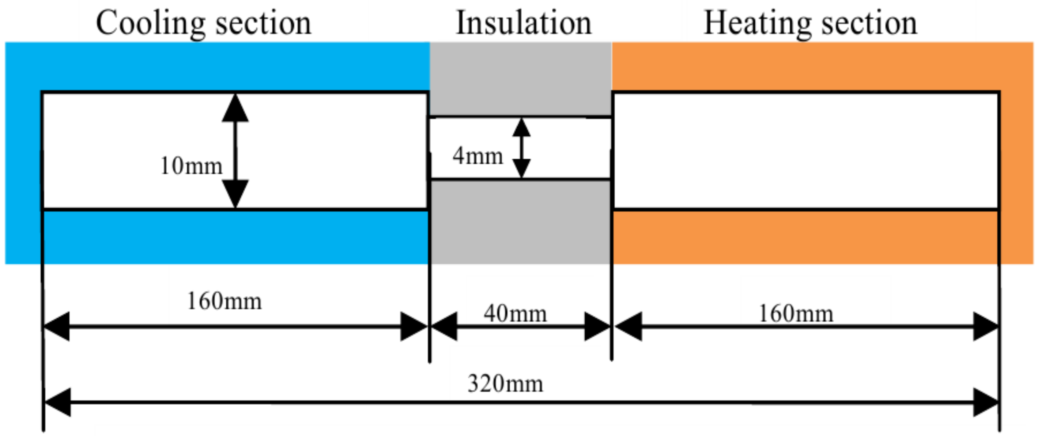
$$\frac{\partial(\rho w_a)}{\partial t} + v \cdot (\rho \nabla w_a) = D_{a,b}\nabla^2(\rho w_a) + D_T w_{a,0}\left(1 - w_{a,0}\right)\nabla^2(\rho T)$$

OpenFOAM Thermodiffusion Solvers Test

- Two cases from ***Kuwatani et. Al 2012*** were selected for testing the new thermodiffusion solvers in OpenFOAM.
- Case 1 closed system:
  - H_2-CO_2 mixture
  - Geometry: Insulated region, with fixed temperature at left and right boundaries.
  - Hexahedral mesh of 3200 elements.
  - Zero flux condition at solid boundaries:

$$\nabla w_a = \frac{D_T}{D_{a,b}}\ w_{a_0}(1 - w_{a_0})\nabla T$$

Simulation	T_c [K]	T_H[K]	$x_{a,0}$	α_T	$D_{a,b}$ [m/s]
1	273.15	473.15	0.48	0.3602	$6.34e^{-5}$
2	----------	523.15	----------	----------	----------
3	----------	573.15	----------	----------	----------
4	----------	593.15	----------	----------	----------
5	----------	693.15	----------	----------	----------
6	----------	723.5	----------	----------	----------
Experiment	313.15	670.15	----------	----------	----------



- Sketch of thermophoresis separation open system, (retrieved from Kuwatani et Al. 2012)

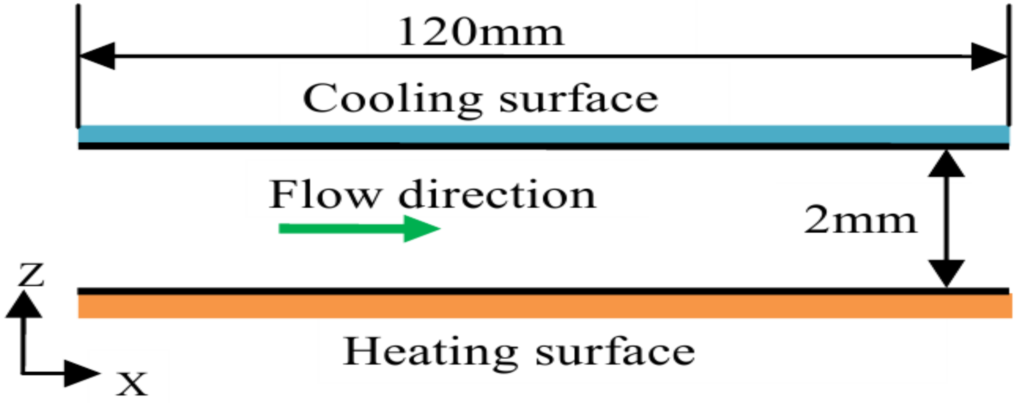
Notice: Molar fraction is converted to mass fraction for species transport equation consistency for both cases.

*Kuwatani, S., Watanabe, S., Ono, N. *Study and Development of a Mini-Tube Gas Separator Utilizing the Soret Effect. 2012. Journal of Thermal Science and Technology. 7(1), 31-43.*

- Case 2 Open system :
  - H2-CO2 mixture.
  - Forced convection, absolute pressure, $\mathrm{P} = 1e^{5}$
  - 6000 hexahedral elements.
  - Zero flux condition at solid boundaries and outlet boundary:

$$\nabla w_a = \frac{D_T}{D_{a,b}} w_{a_0}(1 - w_{a_0})\nabla T$$

Volume flow rate (mL/min)	T_{inlet} [K]	T_c [K]	T_H [K]	$x_{a,0}$
150	300.15	273.15	4	0.5
$D_{a,b}$ $[m/s]$	α_T	μ $[Pa \cdot s]$	$Cp \left[\frac{J}{Kg \cdot K}\right]$	$Pr = \frac{\mu Cp}{\rho \kappa}$
$6.34e^{-5}$	0.3596	$1.02e^{-5}$	1427	0.217



- Sketch of thermophoresis separation open system, (retrieved from Kuwatani et Al. 2012)

CASE 1: CONCENTRATION DIFFERENCE IN THE CLOSED SYSTEM

- Results of the six different steady-state simulations are compared with theoretical calculations and simulations from *Kuwatani et al. 2012. Theoretical calculations are computed by:*

$$\Delta x = -K_T ln\left(\frac{T_h}{T_c}\right)$$

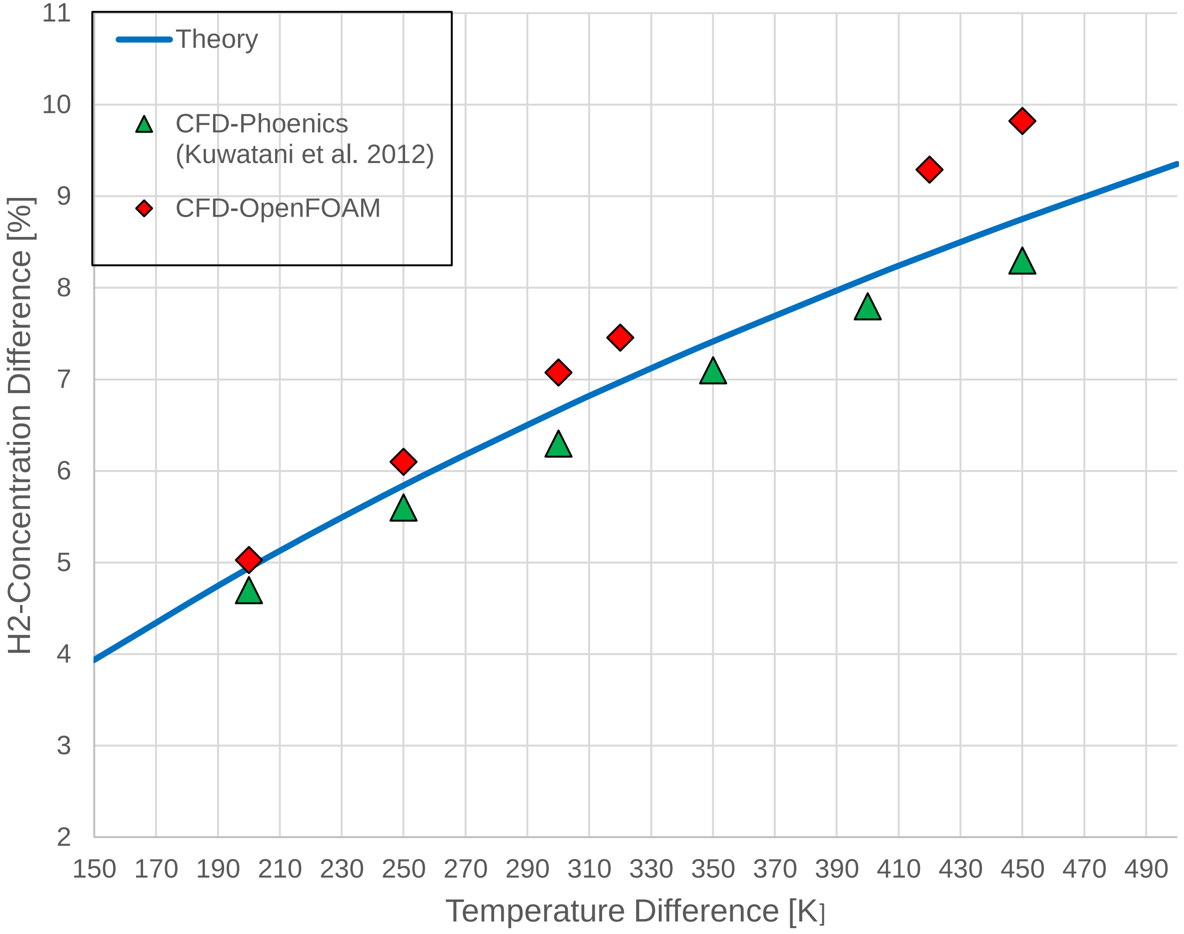
$$K_T = \frac{D_T}{D_{a,b}}T = \alpha_T x_{a,0}\left(1 - x_{a,0}\right)$$

- Comparison with experimental case data (Tc=313.15k, Th=670.15):

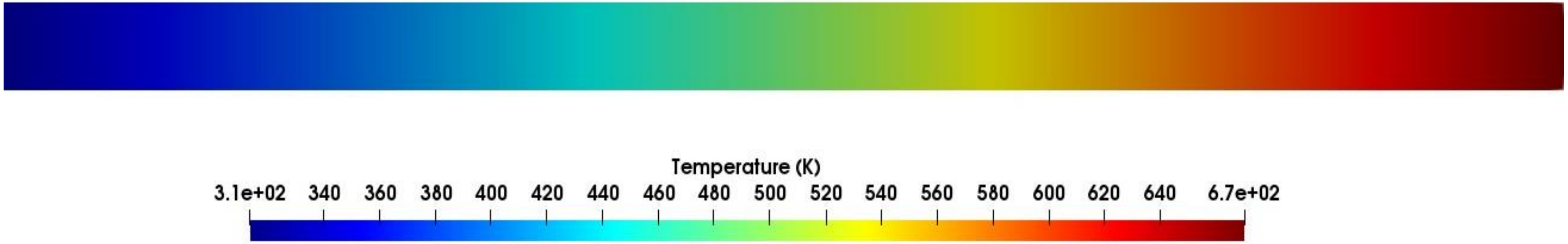
$$\Delta x_{OF} = 7.3\%$$
$$\Delta x_{theory} = 6.8\%$$

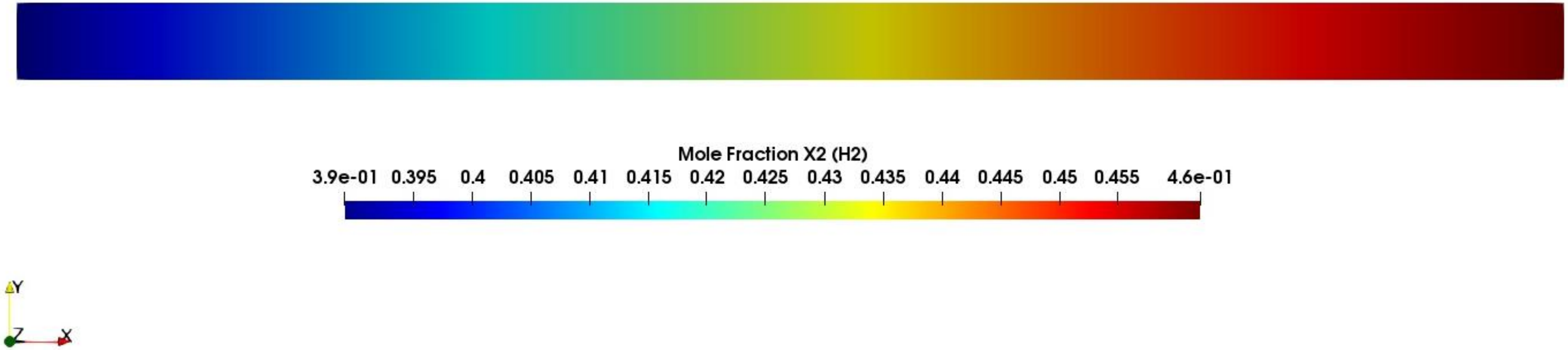
$$\Delta x_{exp} = 6.6\%$$

- Greater differences between OpenFOAM results and theoretical calculations are appreciated for higher temperature differences.



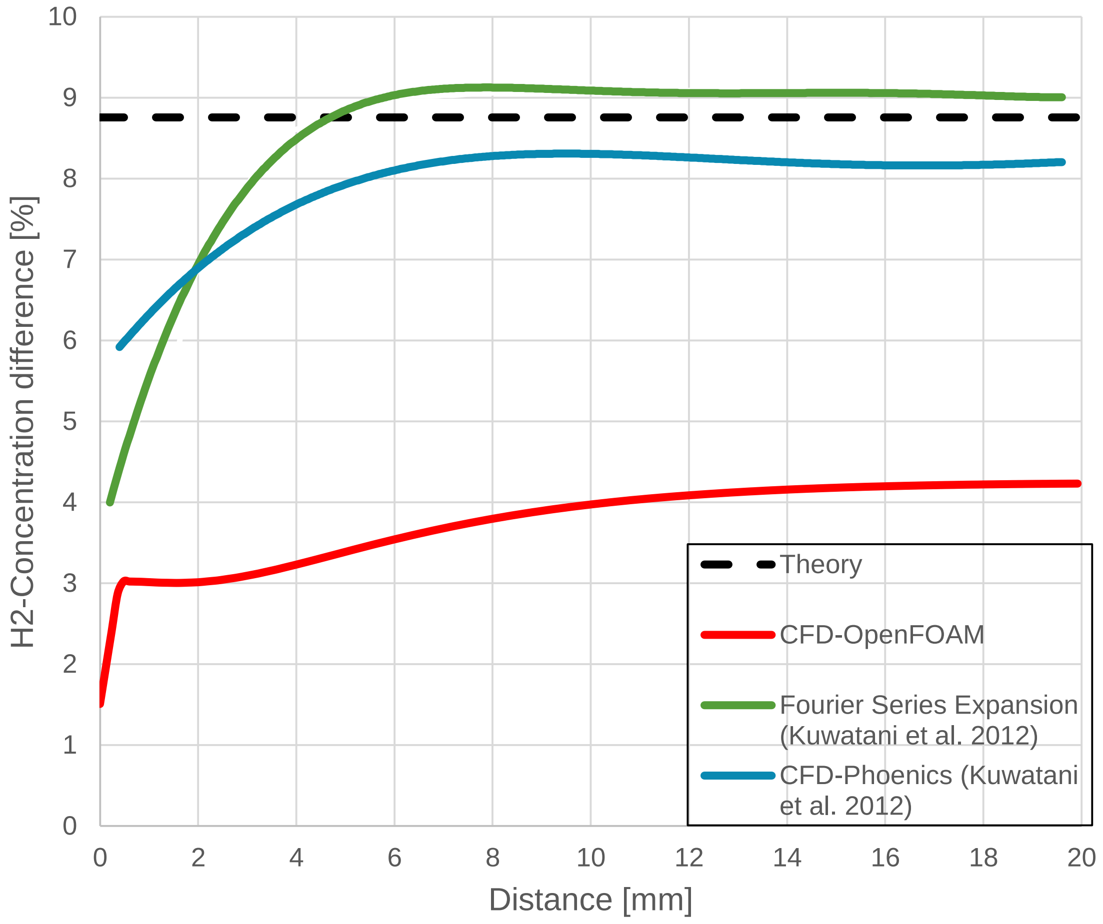
Case 2: Concentration Difference in the Closed System





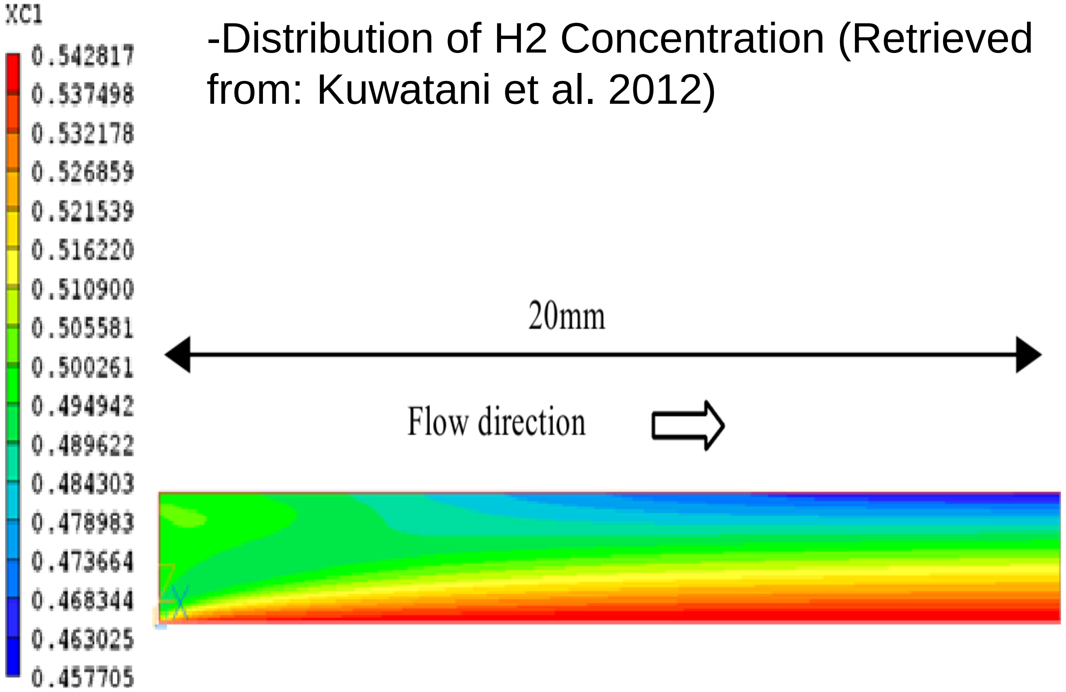
Case 2: Concentration Difference in the Open System

- Qualitative agreement can be observed although the numerical results differ greatly from Kuwatani et al. 2012 reported data.
- Computations were carried out by considering convective terms for transport equations, while theoretical calculations, other CFD results and Series solution does not consider those terms.



CASE 2: CONCENTRATION DISTRIBUTION, OPENFOAM SIMULATION VS. KUWATANI ET AL., 2012

-Distribution of H2 Concentration (Retrieved from: Kuwatani et al. 2012)



-Distribution of H2 Concentration (OpenFOAM).