Single-Cell Chemistry: Introduction

CPFD Software

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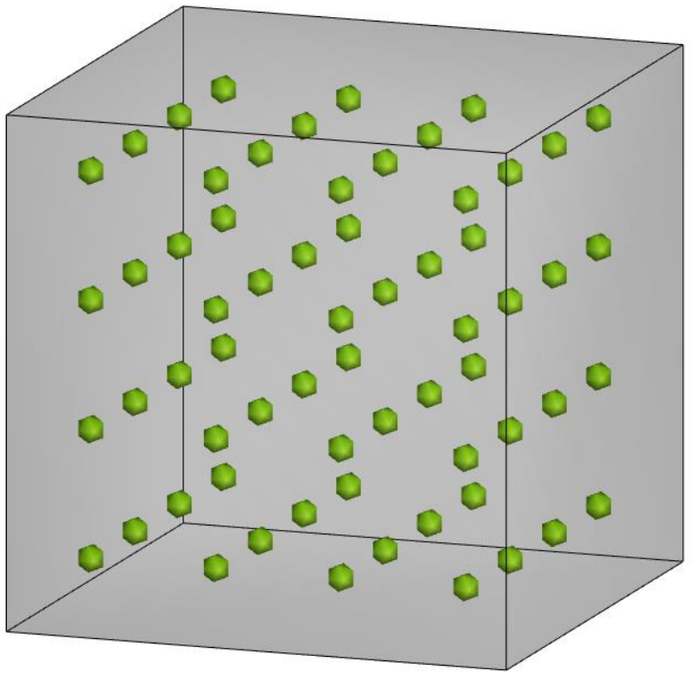
Goals and Objectives

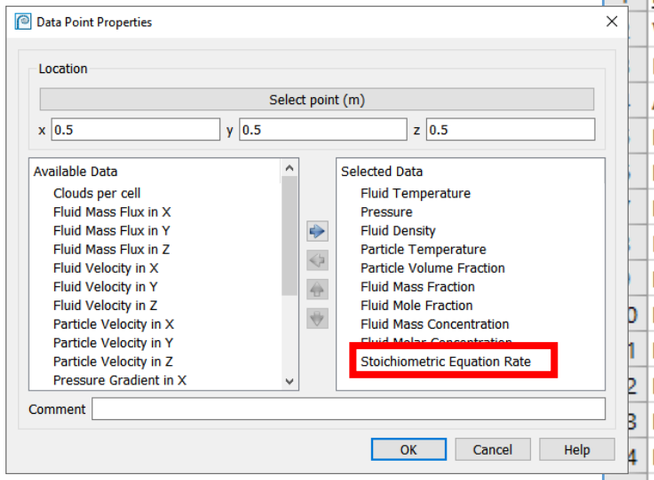
This example shows how to verify that chemistry is input correctly in Barracuda. Concepts introduced include:

- Using a single cell simulation
- Using stationary particles
- Independently calculating expected reaction rates
- Verifying that Barracuda-calculated reaction rates match expected results

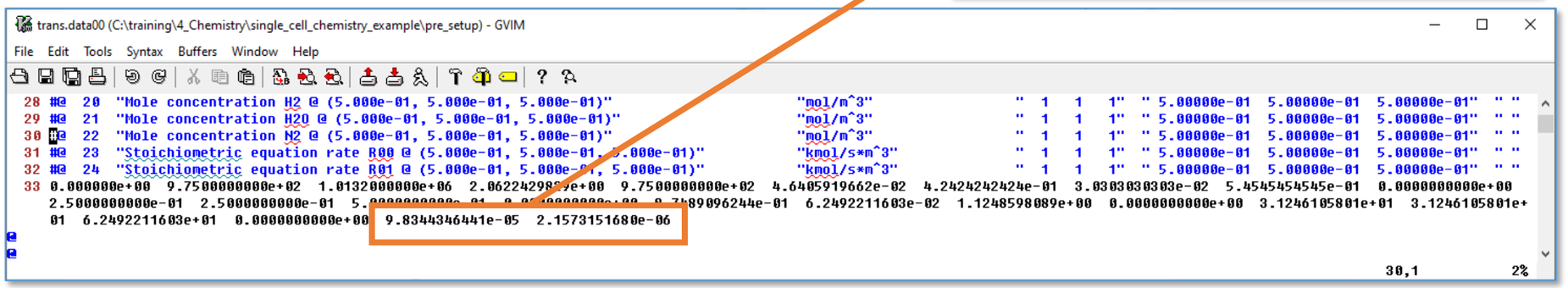


Verify Reaction Rate

Included Spreadsheet (`steam_gasification_hand_calculation.xlsx`) is used to calculate expected reaction rates which are then compared with data point results.



	A	B	C
1	**Initial Conditions in Simulation**		
	Volume of cell	1	m^3
	Fluid temperature	975	K
	Absolute pressure	1.01E+06	Pa
	Mass of particles	100	kg
	Mass fraction of C in particles	0.9	
	Mass concentration of C	90	kg/m^3
	Ideal gas constant	8.3145	J/mol/K
	Mole fraction of H2O	0.50	
10	Mole fraction of H2	0.25	
11	Mole fraction of CO	0.25	
12	Molar concentration of H2O	6.2492E+01	mol/m^3
13	Molar concentration of H2	3.1246E+01	mol/m^3
14	Molar concentration of CO	3.1246E+01	mol/m^3
15			
16	**Hand-calculated Reaction Rates**		
17	Forward reaction, R00	9.8344E-05	kmol/m^3/s
18	Reverse reaction, R01	2.1573E-06	kmol/m^3/s



Import Chemistry

Materials and chemistry can be imported to final case once each piece is verified.