

# Single-Cell Chemistry: Introduction

CPFD Software

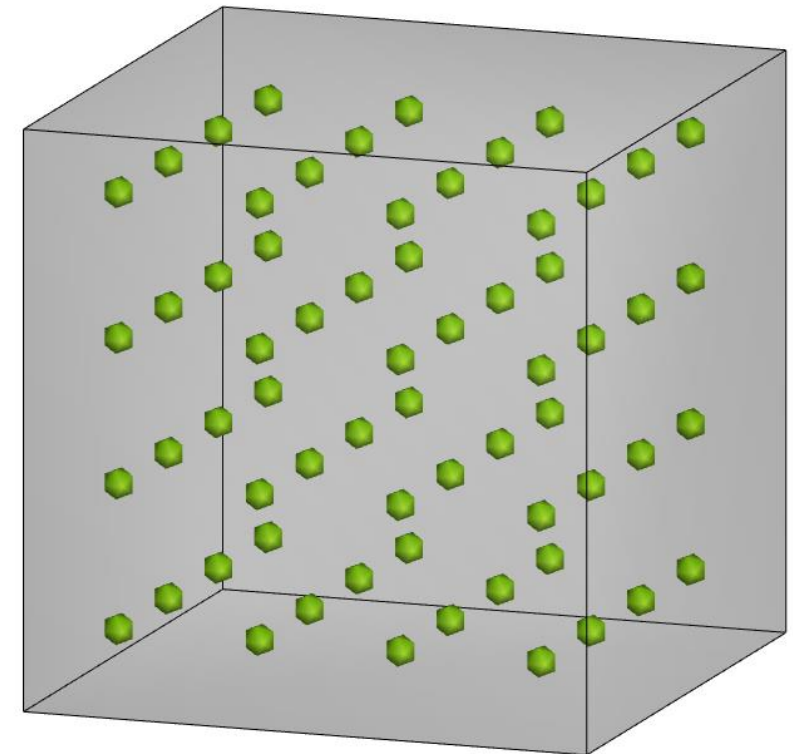
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# Goals and Objectives

**This example shows how to verify that chemistry is input correctly in Barracuda.**

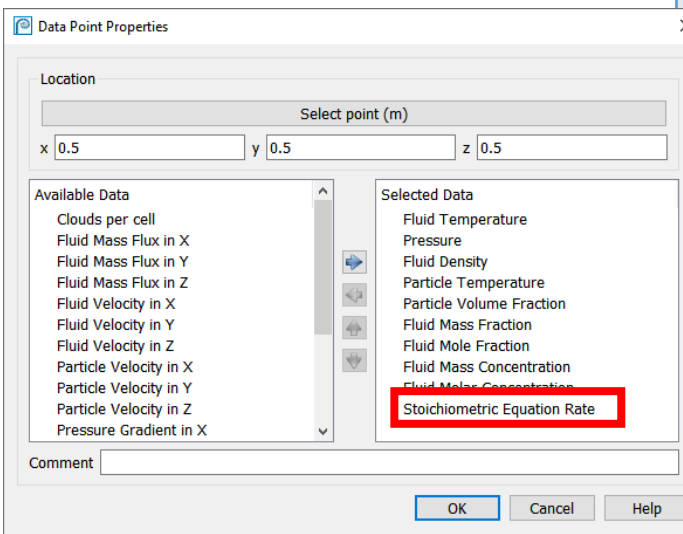
**Concepts introduced include:**

- 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	<b>Initial Conditions in Simulation</b>		
	Volume of cell	1	m <sup>3</sup>
	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 <sup>3</sup>
	Ideal gas constant	8.3145	J/mol/K
	Mole fraction of H <sub>2</sub> O	0.50	
	Mole fraction of H <sub>2</sub>	0.25	
	Mole fraction of CO	0.25	
2	Molar concentration of H <sub>2</sub> O	6.2492E+01	mol/m <sup>3</sup>
3	Molar concentration of H <sub>2</sub>	3.1246E+01	mol/m <sup>3</sup>
4	Molar concentration of CO	3.1246E+01	mol/m <sup>3</sup>
15			
16	<b>Hand-calculated Reaction Rates</b>		
17	Forward reaction, R00	9.8344E-05	kmol/m <sup>3</sup> /s
18	Reverse reaction, R01	2.1573E-06	kmol/m <sup>3</sup> /s

trans.data00 (C:\training\4\_Chemistry\single\_cell\_chemistry\_example\pre\_setup) - GVIM

File Edit Tools Syntax Buffers Window Help

28 #@ 20 "Mole concentration H2 @ (5.000e-01, 5.000e-01, 5.000e-01)" "mol/m^3" " 1 1 1" " 5.00000e-01 5.00000e-01 5.00000e-01" " "

29 #@ 21 "Mole concentration H2O @ (5.000e-01, 5.000e-01, 5.000e-01)" "mol/m^3" " 1 1 1" " 5.00000e-01 5.00000e-01 5.00000e-01" " "

30 #@ 22 "Mole concentration N2 @ (5.000e-01, 5.000e-01, 5.000e-01)" "mol/m^3" " 1 1 1" " 5.00000e-01 5.00000e-01 5.00000e-01" " "

31 #@ 23 "Stoichiometric equation rate R00 @ (5.000e-01, 5.000e-01, 5.000e-01)" "kmol/s\*m^3" " 1 1 1" " 5.00000e-01 5.00000e-01 5.00000e-01" " "

32 #@ 24 "Stoichiometric equation rate R01 @ (5.000e-01, 5.000e-01, 5.000e-01)" "kmol/s\*m^3" " 1 1 1" " 5.00000e-01 5.00000e-01 5.00000e-01" " "

33 0.000000e+00 9.7500000000e+02 1.0132000000e+06 2.062242989e+00 9.7500000000e+02 4.6405919662e-02 4.242424242e-01 3.0303030303e-02 5.4545454545e-01 0.0000000000e+00

2.5000000000e-01 2.5000000000e-01 5.0000000000e-01 0.0000000000e+00 0.0000000000e+00 0.0000000000e+00 0.0000000000e+00 0.0000000000e+00 0.0000000000e+00 0.0000000000e+00

01 6.2492211603e+01 0.0000000000e+00 9.8344346441e-05 2.1573151680e-06

30,1 2%

# Import Chemistry

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

