

MATERIALS STUDIO CANTERA

OVERVIEW

A detailed knowledge of reaction kinetics is required in order to accurately model chemically reacting or combusting systems. These systems are complex, with multiple interdependent reaction pathways and competing processes involved. Reaction kinetics simulations provide predictions for the concentration of reactants and products under a specific set of reactor conditions and geometries.

BIOVIA Materials Studio Cantera is designed to support these calculations by linking thermodynamic input and reaction step data with established Cantera reaction kinetics solvers. In addition, users can supplement existing reaction mechanism data with quantum mechanical transition state calculations, all on a firm, thermodynamically-consistent basis.

BIOVIA Materials Studio Cantera enables scientists and engineers to make predictions covering a diverse range of problems, including exhaust-gas emissions, ignition phenomena, engine knock, flame-speed, flammability limits, catalytic lightoff and chemical conversion. Reaction kinetics simulations for issues in fuel cell development, batteries research, fuel reforming, material deposition and plasma processing research can all be addressed using BIOVIA Materials Studio. New Cantera users can conveniently execute calculation tasks for gas phase reactions and 1D Flame models with Cantera's intuitive user interface, while experts can access the full power of the native Python scripting layer. This combination of ab initio simulation and the Cantera solver provides a unique and powerful set of capabilities for chemists and chemical engineers alike.

WHAT IS CANTERA?

Cantera is a collection of tools from www.cantera.org for addressing problems involving chemical kinetics, thermodynamics and transport processes. Cantera can represent phases of matter, phase-phase interfaces, reaction managers, time-dependent reactor networks and steady one-dimensional reacting flows. The BIOVIA Materials Studio Cantera module allows users to manage the configuration and generation of Cantera input files and execute jobs via the client-server gateway from a dedicated user interface or via MaterialsScript commands.

KEY USES OF CANTERA

Reactor Design, Optimization & Improvement

Cantera allows users to explore the effects of reactor geometry and operating conditions on processes to identify trade-offs, determine reaction controllability and optimize existing reactors.

Identification & Quantification of Emissions

Reaction kinetics simulations may be deployed to understand the byproducts of reactions and predict how process changes can affect the process further downstream.

Sensitivity Analysis

Users of Cantera can better identify dominant chemistry mechanisms and understand experimentally observed results to study and optimize the most promising pathways with further experiments or simulations.

THE BIOVIA MATERIALS STUDIO ADVANTAGE

BIOVIA Materials Studio Cantera is part of BIOVIA Materials Studio modeling and simulation suite. The integrated model building and editing tools enable you to construct, visualize, and manipulate molecular structures. Additionally the ab initio solvers can be deployed to calculate the rate coefficients required for each reaction. For an ordinary reaction, these are the activation energy, a pre-factor, and a temperature exponent.

A BIOVIA Materials Studio DMol³ geometry optimization with a vibrational analysis can be performed first for each species, then the species or reaction can be added to a reaction Study Table using the Cantera Reaction Editor. Alternatively, the species can be taken from the output of a DMol³ Reaction Kinetics task, which performs the optimization and vibrational analysis of all reactants and products automatically.

Accurate combustion simulation requires accurate chemistry and effective simulation reduces development time and cost while fueling innovation. Although industry has embraced CFD simulations with some chemical kinetics, typically the chemical mechanisms are poor and lack the capability to extend with new compounds. Design based on experiment alone cannot address the complex requirements of large chemical kinetic mechanisms.

BIOVIA Materials Studio offers a single environment for the calculation of rate coefficients and their deployment in macroscopic chemical reaction simulation by combining experimental data with accurate ab initio predicted chemistry using:

- 100s of species
- 1000s of reactions
- Fast simulation and setup
- Accurate information about reacting system
- Trace species emissions (parts per billion or smaller)
- Accurate handling of kinetics time and length scales
- Complex dependency between major and minor species
- Dominant reaction paths
- Sensitivity of results to reaction parameters

HOW DOES CANTERA WORK?

For any general chemical reaction, expressed as



the two quantities of interest are the Equilibrium constant, the ratio of reactants to products at equilibrium, and the rate coefficient k , which governs the overall rate of reaction:

$$\frac{d[A]}{dt} = -k[A][B]$$

Reaction	Type	Equation	Standard enthalpy of formation	Prefactor	Temperature exponent	Activation barrier	E
1	fallout_reaction	2 OH (+ M) <=> H2O2 (+ M)	-67.36132159	7.4050000e+013	-0.37000000	0	0
2	reaction	2 H + H2O <=> H2 + H2O	-110.34416957	6.0000000e+019	-1.25000000	0	0
3	reaction	H + 2 O2 <=> HO2 + O2	-50.40554074	2.0000000e+019	-1.24000000	0	0
4	reaction	H + O2 + H2O <=> HO2 + H2O	-50.40554074	1.1260000e+019	-0.76000000	0	0
5	reaction	OH + H2O2 <=> HO2 + H2O	-41.49610170	1.7000000e+018	0	29410	0
6	reaction	H + O2 + AR <=> HO2 + AR	-50.40554074	7.0000000e+017	-0.80000000	0	0
7	reaction	2 H + H2 <=> 2 H2	-110.34416957	9.0000000e+016	-0.60000000	0	0
8	reaction	H + O2 <=> O + OH	44.81796986	2.6500000e+016	-0.67070000	17041	0
9	reaction	OH + H2O2 <=> O2 + H2O	-73.73792315	5.0000000e+015	0	17330	0
10	reaction	2 H2O2 <=> O2 + H2O2	-32.24182145	4.2000000e+014	0	12000	0
11	reaction	H + H2O2 <=> 2 OH	-14.86554110	8.4000000e+013	0	635	0
12	reaction	H + H2O2 <=> O2 + H2	-59.93862882	4.4000000e+013	0	1068	0
13	reaction	O + H2O2 <=> OH + O2	-59.48351097	2.0000000e+013	0	0	0
14	reaction	OH + H2O2 <=> O2 + H2O	-73.73792315	1.4500000e+013	0	-500	0
15	reaction	H + H2O2 <=> OH + H2O	-56.16164280	1.0000000e+013	0	3600	0
16	reaction	H + H2O2 <=> O + H2O	-28.91995328	3.9700000e+012	0	671	0
17	reaction	OH + H2O2 <=> HO2 + H2O	-41.49610170	2.0000000e+012	0	427	0
18	reaction	2 H2O2 <=> O2 + H2O2	-32.24182145	1.3000000e+011	0	-1630	0
19	reaction	OH + H2 <=> H + H2O	-13.79929433	2.1600000e+008	1.51000000	3430	0
20	reaction	H + H2O2 <=> HO2 + H2	-27.69680737	1.2100000e+007	2	5200	0
21	reaction	O + H2O2 <=> OH + HO2	-27.24188952	9.6300000e+006	2	4000	0

Figure 1: Reaction tab from a BIOVIA Materials Studio Reaction Study Table

For a system of reactions, Cantera will solve for concentrations as a function of time and/or space within the constraints set by the reaction vessel conditions. The Cantera solver itself offers considerable flexibility via a Python scripted interface.

Most realistic simulations of interest will contain multiple species and reactions. An example scheme for hydrogen combustion (Figure 1) could be considered a relatively simple reaction; however, it requires a large amount of thermodynamic and transport data to characterize the input species and rate information must be given for each fundamental reaction step. BIOVIA Materials Studio Cantera provides a convenient framework for managing this input and executing the calculations.

Reaction Vessels

Reactors can interact with the surrounding environment in multiple ways, including expansion/compression work and heat or mass transfer. All of these interactions can also vary as a function of time or state. For example, heat transfer can be described as a function of the temperature difference between the reactor and the environment, or the wall movement can be modeled depending on the pressure difference. Typically, interactions of the reactor with the environment are defined on one or multiple walls, inlets, and outlets.

With Python script single reactors may be also connected to form a Reactor Network such that the contents of one reactor flow into another or contact one another or the environment via walls which move or conduct heat.

Preparing Reaction Study Tables

BIOVIA Materials Studio Cantera uses a study table containing details of the species and reactions involved in the calculation as the primary input. Each species must be accompanied by its transport properties and thermodynamic information, namely its enthalpy, entropy, and heat capacity as a function of temperature, represented as a NASA polynomial.

Modifying Reaction Study Tables: The Reaction Editor

The Cantera Reaction Editor dialog allows you to create and modify reaction Study Tables defining the reaction mechanism. It automatically recognizes molecules and reactions which are already present in the mechanism allowing you to quickly validate input. It also calculates or updates NASA polynomials where required to meet the new standard state definitions. The Reaction Editor also includes support for importing gas-surface reaction rate data created using the DMol3 Reaction Kinetics task.

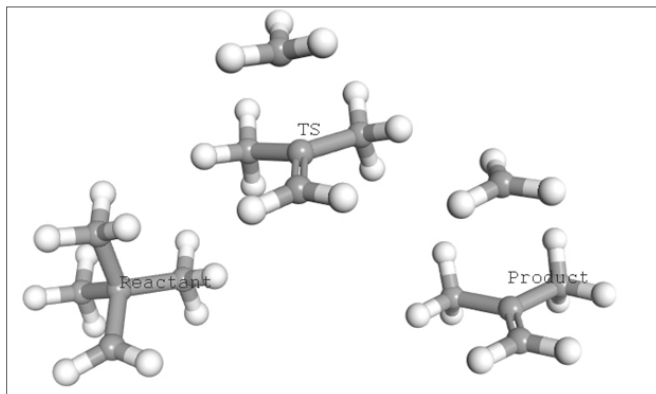


Figure 2: Reaction, transition state and products from the dissociation of neopentyl radical to generate reaction rate input using BIOVIA Materials Studio DMol³.

KEY FEATURES

- Model chemically reacting or combusting systems using detailed reaction mechanisms.
- Connect ab initio calculations and reaction kinetics simulations within the same Materials Studio project
- Supports reactions at surfaces

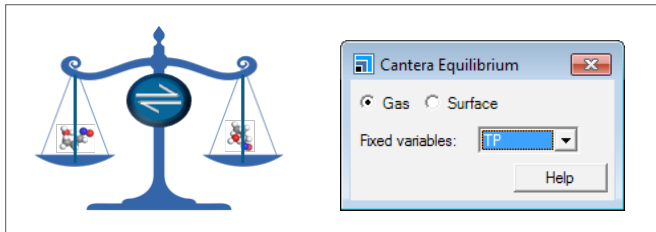


Figure 3: The Cantera Equilibrium Task calculates the final composition of a reaction at thermodynamic equilibrium based on initial reactant concentration, temperature and pressure.

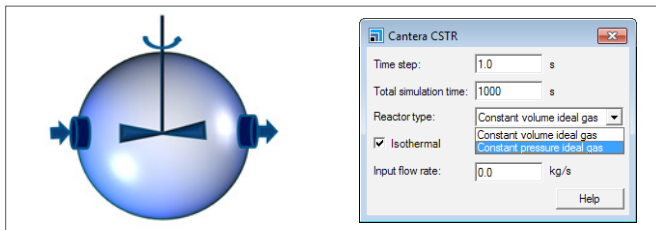


Figure 4: The Cantera CSTR task determines the concentration of products within a continuous stirred-tank reactor as a function of time based on reactant concentrations.

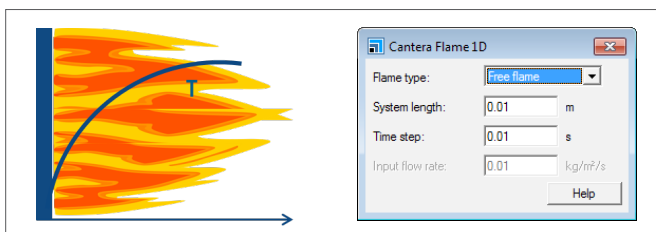


Figure 5: The Cantera Flame1D task calculates the concentration of products as a function of position as well as the velocity of the propagating flame from reactant concentration, temperature and pressure.

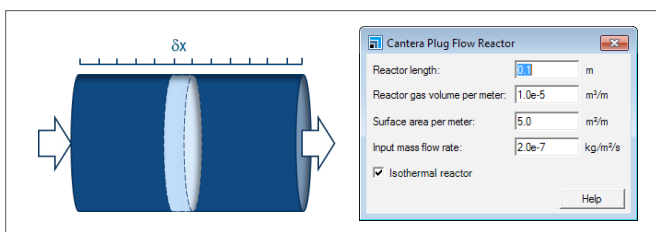


Figure 6: The Cantera Plug Flow Reactor calculates the concentration of products as a function of position along the reactor using reactant concentrations, temperature and pressure and takes into account the proportion of surface reactive sites on the internal surface.

- Cantera Calculation for selected tasks
 - Equilibrium - calculates the composition of a mixture at thermodynamic equilibrium, including surface coverage prediction
 - CSTR - performs a continuous stirred-tank reactor simulation
 - Flame1D - performs a one-dimensional flame calculation
- Plug Flow reactor - perform modeling of gas flows, including across reactive surfaces
- Cantera Reaction Editor
 - for validating reaction mechanism input
 - for re-calibrating ab initio data to be thermodynamically consistent
- Full access to native Cantera Python scripts for expert users
- Tutorials describing typical workflows for all major Cantera tasks

Running Jobs

- All BIOVIA Materials Studio Cantera jobs are run in the background freeing up the BIOVIA Materials Studio client for other research.
- All BIOVIA Materials Studio Cantera jobs can be submitted to remote high performance compute servers.

To learn more about BIOVIA Materials Studio, go to 3dsbiovia.com/materials-studio

REFERENCES

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