Kintecus–Excel Workbook Library

A Chemical-Engineering Description of Each Worksheet

87 workbooks · organized by application area

Introduction

This document describes each Kintecus-Excel workbook in the supplied collection and explains how it is used from a chemical-engineering standpoint. Where a direct chemical-engineering or water-chemistry application exists it is given; where it does not, the nearest physical-chemistry or pedagogical use is provided instead.

Every workbook follows the same Kintecus structure. A model sheet lists the elementary reactions and their rate parameters (either a single rate constant k, or the extended Arrhenius triple A, T^m, Ea); a species sheet lists each chemical species with its initial concentration, residence time in a CSTR, and output flags; and CONTROL, parm and (for combustion cases) therm and TRANSPORT sheets hold the run settings, integration parameters, thermodynamic polynomials and transport data. Workbooks ending in additional sheets such as FITPLOT/FDATA, mp1/d1, SENSIT, SCANPLOT or CONCMIN/MAX/AVG support regression fitting, sensitivity analysis, parameter scanning and uncertainty (confidence-band) analysis respectively.

From a process standpoint, each workbook is effectively a zero-dimensional reactor model: an isothermal or non-isothermal batch reactor, a continuous stirred-tank reactor (when a residence time is set), or a variable-volume reactor (when a volume or temperature profile is supplied). The same mass-action machinery is applied across combustion, water treatment, biocatalysis, polymerization, equilibrium thermodynamics and several teaching analogies.

Where a workbook carries a descriptive text box on its CONTROL (or species, model or output) worksheet, that author-supplied description has been read and incorporated. It appears in italics beneath the system description as a “Workbook note” and typically supplies the original literature citation, the LLNL/NUI mechanism identifier, or the specific Kintecus feature the workbook was built to demonstrate. The 26 workbooks whose only floating shapes are command buttons or settings boilerplate carry no such note; their descriptions are inferred from the reaction and species sheets.

Contents

1. Combustion & High-Temperature Reaction Engineering

38 workbooks in this group.

Workbook	Chemical system & model	Engineering / applied use
`AramcoMech2.0__HAS_PLOG.xls`	AramcoMech 2.0 detailed combustion mechanism (C0-C4 hydrocarbons, oxygenates) with pressure-dependent PLOG rate expressions and full Chemkin-style thermodynamic (therm) and transport (TRANSPORT) data. Built on the H2/O2 sub-mechanism. *Workbook note: AramcoMech 2.0, NUI Galway Combustion Chemistry Centre (Saudi Aramco funded), downloaded July 2016 from c3.nuigalway.ie. Built hierarchically from an H2/O2 sub-mechanism upward to characterise C1–C4 hydrocarbons and oxygenated fuels over a wide range of conditions.*	Reference foundational mechanism for combustion reactor design and engine simulation. Used to predict ignition delay, laminar flame behaviour and species profiles across the pressures/temperatures encountered in gas turbines and IC engines, where PLOG handles falloff between low- and high-pressure rate limits.
`AramcoMech3.0__HAS_PLOG.xls`	AramcoMech 3.0, the expanded successor mechanism with refined rate parameters and additional fuel sub-mechanisms, again carrying PLOG pressure dependence plus therm/transport tables. *Workbook note: NUI Galway AramcoMech series (the workbook's own text box was copied from the 2.0 file and still reads "AramcoMech 2.0"; the file name and contents are the 3.0 update).*	State-of-the-art validation mechanism for combustion engineers: benchmarking burner, engine and flow-reactor models, and providing the kinetic backbone when reducing large mechanisms for CFD.
`Combustion_H2_O2_cluster.xls`	The branched-chain H2/O2 mechanism used as the dataset for Kintecus's clustering-analysis feature (the -cluster switch), here clustering on a correlation similarity matrix. *Workbook note: this example demonstrates the clustering-analysis feature in Kintecus V3.9 (the -cluster switch), here using a correlation similarity matrix.*	Demonstrates kinetics-driven clustering analysis: grouping species/profiles by similarity of their concentration trajectories — a diagnostic for identifying co-evolving species and lumping candidates during mechanism reduction.
`Combustion_H2_O2_scan.xlsm`	Same H2/O2 mechanism set up to scan an input parameter (here the O2 initial concentration is bracketed for sweeping). *Workbook note: demonstrates the parameter-scanning feature (-scan:1 switch); here scanning a single parameter, the O2 concentration.*	Parametric reactor study: sweeping feed stoichiometry/equivalence ratio to locate ignition thresholds and optimum operating windows, a standard combustion-engineering screening exercise.

Workbook	Chemical system & model	Engineering / applied use
`Combustion_H2_O2_sensit.xlsm`	H2/O2 mechanism configured for normalized sensitivity analysis of species concentrations with respect to each rate constant. *Workbook note: demonstrates normalized sensitivity analysis (NSA) plotting (-SENSIT switch, uppercase required).*	Identifies the rate-controlling elementary steps so designers know which kinetics dominate ignition and heat release — the basis for rational mechanism reduction before CFD reactor modelling.
`Combustion_H2_O2_sensit_AT_TEST.xlsm`	H2/O2 sensitivity workbook with 31 stored SENSIT result sheets (time-resolved sensitivity coefficients) for post-processing. *Workbook note: NSA plotting at user-selected time intervals (see O_sens.txt).*	Demonstrates time-dependent sensitivity output for combustion diagnostics, letting engineers see how the controlling reaction shifts through induction, branching and burnout phases.
`Combustion_OH_DYNAMIC.xls`	H2/O2 (OH-producing) mechanism with a dynamic-condition sheet driving time-varying temperature/volume during the run. *Workbook note: uses the Dynamic Kintecus worksheet (dyn_plot); only finalized, completed mechanisms should be placed in it.*	Models combustion under non-isothermal, time-varying reactor conditions such as compression/expansion strokes or programmed heating — directly relevant to engine-cylinder and rapid-compression-machine simulation.
`Combustion_workbook_OH.xlsm`	Baseline H2/O2 OH-chemistry workbook with temperature and concentration output sheets; the reference template the other OH variants build on.	Teaching/working template for setting up an adiabatic or isothermal combustion batch reactor and reading out temperature and radical-pool evolution.
`Combustion_workbook_OH_CONF.xlsm`	OH combustion model with confidence-interval output sheets (CONCMIN/CONCMAX/CONCAVG/CONCSTD) from Monte-Carlo style runs. *Workbook note: confidence/uncertainty run; author notes the integrator accuracy may need tightening (~1e-8) on some processors.*	Propagates rate-constant uncertainty into predicted concentration bands — essential for risk-aware combustor and safety-margin design.
`Combustion_workbook_OH_enthalpy_fit.xlsm`	OH combustion model set up to regress thermodynamic (enthalpy) parameters against data, with THERMOUT and FITPLOT sheets. *Workbook note: regresses the initial concentration of a species (O2 here) against the measured heat (enthalpy) output of an experiment.*	Lets an engineer refine species thermochemistry (heats of formation / NASA polynomials) from measured profiles, improving energy-balance accuracy in reactor heat-release predictions.
`Combustion_workbook_OH_multifit.xlsm`	OH combustion model configured to fit several rate constants simultaneously against three datasets (d1/d2/d3, multi-plot). *Workbook note: multi-dataset fit of activation energies (Ea) across three datasets at different initial*	Global kinetic parameter estimation from multiple experiments at once — the standard way to obtain self-consistent Arrhenius parameters for design-grade mechanisms.

Workbook	Chemical system & model	Engineering / applied use
	conditions (1000/1500/1700 K); see O_initconditions.txt.	
`Combustion_workbook_OH_props.xlsm`	OH combustion model exporting derived properties: per-reaction rates (SPECRATE/RATESOUT), thermodynamic output and full system output (SYSOUT). *Workbook note: outputs full system thermodynamics and reaction properties via the -o:y:y:y:y switch.*	Generates reaction-flux and thermochemical property tables used for flux analysis and reactor energy balances.
`Combustion_workbook_OH_user_defined_functions.xlsm`	OH combustion model where several rate laws are replaced with USER-defined symbolic expressions (custom k = f(T, concentrations)).	Shows how to embed non-standard or empirical rate forms (e.g. custom falloff, third-body weighting) — useful when a process exhibits kinetics outside the Arrhenius template.
`Combustion_BIODIESEL2_CH3C10_C7_surrogate.xls`	Biodiesel surrogate mechanism (methyl-decanoate-type ester + n-heptane co-fuel) with large C0-C10 hydrocarbon/oxygenate set, therm and transport data. *Workbook note: Herbinet, Pitz & Westbrook (LLNL), biodiesel surrogate = Methyl Decanoate + n-Heptane, v2, LLNL-MI-415050 (Combustion and Flame, 2009). ~5 h runtime on a Core i7.*	Predicts ignition and emissions behaviour of biodiesel blends for compression-ignition engine and burner design and renewable-fuel evaluation.
`Combustion_BIODIESEL_CH3-9-C10_C7_surrogate.xls`	Alternate biodiesel surrogate (methyl-ester + n-heptane) detailed mechanism in explicit forward/reverse Arrhenius form. *Workbook note: Herbinet, Pitz & Westbrook (LLNL), surrogate = Methyl-9-Decenoate + Methyl Decanoate + n-Heptane, LLNL-MI-415050 (Combustion and Flame, 2009). ~2 h runtime.*	Companion biodiesel surrogate for comparing fuel-structure effects on autoignition and soot precursors in engine combustion studies.
`Combustion_C8_to_C16_alkanes.xls`	Detailed oxidation mechanism spanning C8-C16 normal alkanes (n-decane representative fuel) with TROE falloff and transport data. *Workbook note: Westbrook, Pitz, Herbinet, Curran & Silke, "A Detailed Chemical Kinetic Reaction Mechanism for n-Alkane Hydrocarbons from n-Octane to n-Hexadecane," Combust. Flame (2008); LLNL n-alkane mechanisms v2.*	Surrogate kinetics for kerosene/jet and diesel-range fuels; used to design and optimize gas-turbine and diesel combustors and to study cetane behaviour.
`Combustion_DIESEL_surrogate.xls`	Full diesel surrogate combustion mechanism (large-alkane + aromatic blend) with explicit reverse reactions, therm and transport tables.	Engine-relevant diesel autoignition and emissions modelling for compression-ignition combustion-chamber design.

Workbook	Chemical system & model	Engineering / applied use
	Workbook note: detailed low- and high-T mechanism for species up to C12 + xylenes; Mehl, Sarathy, Westbrook & Pitz (LLNL), Xylene+C12_v1.mech, 2012.	
`Combustion_DIESEL_surrogate_reduced_model.xls`	A reduced (skeletal) version of the diesel surrogate mechanism with original Chemkin lines retained as comments for traceability. *Workbook note: downloaded from LLNL (combustion.llnl.gov diesel-surrogate detailed-and-reduced) July 2016.*	Demonstrates mechanism reduction — trimming species/reactions to a CFD-affordable skeletal model while preserving ignition behaviour, a core combustion-engineering task.
`Combustion_GASOLINE_surrogate.xls`	Gasoline surrogate mechanism built around iso-octane (IC8H18) and companion reference fuels, with therm/transport data. *Workbook note: Mehl, Pitz, Westbrook & Curran, "Kinetic Modeling of Gasoline Surrogate Components and Mixtures under Engine Conditions," Proc. Combust. Inst. 33 (2011) 193-200; LLNL gasoline surrogate v1.0.*	Spark-ignition engine knock and octane-rating studies; surrogate-fuel modelling for SI combustion-chamber optimization.
`Combustion_isooctane3.xls`	Iso-octane (2,2,4-trimethylpentane) detailed oxidation mechanism, the primary high-octane reference fuel. *Workbook note: Iso-octane Model 3, Mehl, Curran, Pitz & Westbrook (LLNL), 2009; LLNL-MI-421507.*	Defines the knock-resistant end of the octane scale; used for SI-engine autoignition/knock prediction and as an RON reference in fuel design.
`Combustion_methlycarbonate.xls`	Dimethyl carbonate / methyl-carbonate oxygenated-fuel combustion mechanism. *Workbook note: Glaude, Pitz & Thomson, "Chemical Kinetic Modeling of Dimethyl Carbonate in an Opposed-Flow Diffusion Flame," Proc. Combust. Inst. 30 (2004) 1095-1102; UCRL-CONF-201358.*	Evaluates oxygenated fuel additives that suppress soot; relevant to clean-diesel and additive-formulation engineering.
`Combustion_methlydecanoate.xls`	Methyl decanoate combustion mechanism — a realistic methyl-ester representative of biodiesel. *Workbook note: Herbinet, Pitz & Westbrook (LLNL), Methyl Decanoate v2, LLNL-MI-415050 (Combustion and Flame, 2009). ~3 h runtime on a Core i7.*	Benchmark biodiesel-component kinetics for renewable-fuel combustor and engine design.
`Combustion_Organophosphates.xls`	Hydrocarbon combustion mechanism extended with organophosphorus chemistry (H/O/C1/C2 core plus P-species).	Models flame inhibition/suppression by phosphorus agents and incineration of organophosphate compounds — fire-suppression and hazardous-waste-destruction engineering.

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	Workbook note: Glaude, Melius, Pitz & Westbrook, "Detailed Chemical Kinetic Reaction Mechanisms for Incineration of Organophosphorus and Fluoro-Organophosphorus Compounds," Proc. Combust. Inst. 29 (2002) 2469-2476; UCRL-JC-146563.	
`Combustion_TNT_and_RDX.xls`	Combustion/decomposition mechanism for energetic materials (TNT and RDX) built on a C/H/O/N hydrocarbon core. *Workbook note: Pitz & Westbrook, "A detailed chemical kinetic model for gas phase combustion of TNT," Proc. Combust. Inst. 31 (2007) 2343-2351; LLNL mechanism tnt_v1j_tol_v6k_rdx_1a_c4_2c.mech.*	Energetic-material decomposition and afterburn modelling for propulsion, demilitarization and explosion-safety analysis.
`Ethanol_Combustion.xls`	Ethanol oxidation mechanism (Marinov-type rate data) with LIN/falloff third-body handling.	Bioethanol and flex-fuel combustion modelling for engine and burner design with a renewable oxygenate.
`Dimethylether_combustion.xlsm`	Dimethyl ether (DME) wide-range oxidation mechanism (Curran et al.) with TROE falloff and free-format thermo. *Workbook note: DME combustion example (~10 min on a Pentium IV).*	DME is a clean compression-ignition fuel; this models its low-temperature ignition for alternative-fuel engine design.
`Dimethoxy_model.xlsm`	Dimethoxymethane (DMM/methylal) oxidation mechanism (Daly thesis) with free-format thermodynamic data. *Workbook note: dimethoxymethane combustion example (~3 min on a Pentium IV).*	Oxygenated diesel-additive combustion modelling aimed at soot reduction in compression-ignition engines.
`Heptane_Combustion_Pitz.xlsm`	n-Heptane counterflow ignition/extinction mechanism (Seiser/Pitsch/Pitz/Curran). *Workbook note: uses -obeymaxint with a small maximum integration time for a smoother output curve (~3 min on a Pentium IV).*	n-Heptane is the zero-octane diesel reference fuel; used for autoignition, ignition-delay and extinction-strain studies in CI-engine design.
`n-buthane-combustion.xlsm`	n-Butane oxidation mechanism (Marinov rate data, LIN third-body falloff).	LPG/butane combustion modelling for burners and small engines.
`pitz_propane_model.xlsm`	Detailed propane oxidation mechanism (Curran/Pitz/Westbrook) in explicit forward/reverse form.	Propane/LPG combustor and flame modelling; a common reference for C3 oxidation kinetics.
`GRI_MECH_30.xlsm`	GRI-Mech 3.0 — the 53-species/325-reaction natural-gas (methane) combustion mechanism	The industry-standard methane/natural-gas mechanism for gas-turbine, boiler and burner

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	with NOx, third-body efficiencies and its own thermo file. *Workbook note: the gritherm.dat Chemkin thermodynamic database was converted into the O_gritherm.dat worksheet using the -OF switch.*	design and for validating CFD combustion codes.
GRMECH_with_compression.xlsm	GRI-Mech 3.0 driven by a sinusoidal volume profile (O_sine1.txt) simulating piston compression. *Workbook note: GRI-Mech 3.0 with compression (~20 min on a Pentium IV).*	Couples detailed methane kinetics to engine-cylinder volume change — homogeneous-charge / HCCI-style engine autoignition modelling.
GRMECH_with_compression_heat_loss.xlsm	As above but adding an external wall-temperature profile (O_externtemp.txt) for heat loss during compression. *Workbook note: GRI-Mech 3.0 with compression and heat loss (~15 min on a Pentium IV).*	Adds non-adiabatic heat transfer to the engine-compression model — more realistic cylinder energy balance for IC-engine simulation.
Kilpinen_97_NH3_ORG.xlsm	Kilpinen-97 detailed NH3/NO/O2 nitrogen-chemistry mechanism (Abo Akademi). *Workbook note: Kilpinen 97 NH3/NO/O2 scheme; author notes the integrator accuracy may need tightening on some processors.*	Ammonia combustion and fuel/thermal-NOx formation modelling — central to carbon-free NH3 fuel engineering and combustion NOx control.
nox_model.xlsm	Marinov NO-NO2 conversion mechanism showing hydrocarbon promotion of NO oxidation in a flow reactor.	Flue-gas NOx chemistry for emissions prediction and abatement design in furnaces and engines.
H2-O2-Combustion-gas-liquid-catalytic-surface-tests.xlsm	H2/O2 combustion mechanism configured to test coupled gas-phase, liquid-phase and catalytic-surface reaction handling.	Demonstrates multiphase / heterogeneous-catalytic reaction modelling (gas + surface) relevant to catalytic combustors and surface-reaction reactor design.
Calculate_a_volume_factor_for_pistons.xls	A utility spreadsheet converting a measured piston swept-volume-vs-time profile into the per-step Kintecus volume factor.	Pre-processing tool that turns an engine/rapid-compression-machine volume trace into the time-dependent volume input a variable-volume reactor model needs.
Wolfrum_with_Temp_Program.xlsm	Temperature-programmed desorption of CO from a tungsten crystal (Houle & Hinsberg) using extended Arrhenius with a programmed temperature ramp (O_tempprof.txt).	Surface-science / heterogeneous-catalysis kinetics: extracting desorption activation energies from TPD — directly applicable to catalyst characterization and surface reaction engineering.

2. Water Chemistry & Water-Treatment Engineering

11 workbooks in this group.

Workbook	Chemical system & model	Engineering / applied use
Fe(VI)+ABTS_Fe(IV)_involved_multiple_fitting_20180724_100mM phosphate_pH=7_ks3=1e6.xlsm	Ferrate(VI) oxidation of the ABTS probe via Fe(V)/Fe(IV) intermediates, fitted to four datasets simultaneously; this version in 100 mM phosphate buffer, pH 7. *Workbook note: bootstrapped error analysis of several rate parameters across multiple datasets/initial conditions; results in Huang et al. (ACS); 100 mM phosphate, pH 7 (~12 h runtime).*	Quantifies high-valent iron oxidation kinetics used in ferrate-based drinking-water and wastewater treatment; the buffer/concentration variants probe matrix effects on disinfection/oxidation performance.
Fe(VI)+ABTS_Fe(IV)_involved_multiple_fitting_20180724_10mM phosphate_pH=7_ks3=1e6.xlsm	Same ferrate(VI)/ABTS Fe(IV)-involved kinetic model, 10 mM phosphate buffer, pH 7, multi-dataset fit. *Workbook note: same bootstrapped multi-dataset error analysis (Huang et al., ACS); 10 mM phosphate, pH 7 (~8 h runtime).*	Tests buffer-strength (phosphate) effect on ferrate oxidation rates — water-treatment process design under realistic ionic conditions.
Fe(VI)+ABTS_Fe(IV)_involved_multiple_fitting_20180729_10mM borate_pH=7_ks3=1e6.xlsm	Ferrate(VI)/ABTS Fe(IV)-involved model in 10 mM borate buffer, pH 7, multi-dataset fit. *Workbook note: same bootstrapped multi-dataset error analysis (Huang et al., ACS); 10 mM borate, pH 7 (~17 h runtime).*	Compares borate vs phosphate buffering on ferrate decay/oxidation — supports buffer selection and rate prediction in ferrate water-treatment trains.
Micropollutant Degradation by Ferrate FeVI-PAA.xlsm	Ferrate(VI) + peracetic acid (PAA) system with the full Fe(VI)/Fe(V)/Fe(IV)/Fe(III)/Fe(II) redox cycle and H2O2/O2 side chemistry degrading a micropollutant. *Workbook note: from Wang, Kim, Ashley, Sharma & Huang, "Peracetic Acid Enhances Micropollutant Degradation by*	Models an advanced ferrate/PAA oxidation process for removing trace organic micropollutants (pharmaceuticals, etc.) in water-treatment engineering.

Workbook	Chemical system & model	Engineering / applied use
	Ferrate(VI)...," Environ. Sci. Technol. 56(16) 2022, 11683-11693.	
Superfast degradation of micropollutants in water final.xlsm	Chlorine-dioxide / sulfite radical-chain advanced reduction-oxidation network (ClO2, SO3*-, SO4*-, ClO*, etc.) degrading micropollutants. *Workbook note: from Li et al., "Superfast degradation of micropollutants in water by reactive species generated from the reaction between chlorine dioxide and sulfite," Water Research 222 (2022) 118886.*	Radical-based advanced oxidation/reduction process (AOP/ARP) design for rapid micropollutant destruction in water treatment.
UV_bromine_final_Lee et al., ES&T, 2020.xlsm	UV/bromine advanced-oxidation mechanism (Lee et al., ES&T 2020): photolysis of HOBr/OBr- generating reactive bromine and OH radicals. *Workbook note: from Lee, Lee, Allard, Ra, Han & Lee, "...UV254 Photolysis of Chlorine and Bromine Species in Water and Formation of Oxyhalides," Environ. Sci. Technol. 54(18) 2020; simulates oxidant decay, probe degradation and ClO3-/BrO3- formation.*	Designs UV/bromine AOP and predicts reactive-bromine speciation and bromate formation risk in disinfection — key water-quality engineering concern.
UV_chlorine_final_Lee et al., ES&T, 2020.xlsm	UV/chlorine AOP mechanism (Lee et al., ES&T 2020): photolysis of HOCl/OCl-/ozone producing OH, Cl, O radicals and reactive species. *Workbook note: from Lee et al., Environ. Sci. Technol. 54(18) 2020 (same study as the UV/bromine workbook); simulates oxidant decay, probe degradation and oxyhalide formation.*	Models the widely used UV/chlorine advanced-oxidation process for micropollutant removal and disinfection-byproduct prediction in potable-water treatment.
Water Purification HOCl_chlorite_model.xlsm	Aqueous chlorine/chlorite/chlorine-dioxide disproportionation and	Predicts chlorine-species speciation and chlorate/chlorite byproduct formation during

Workbook	Chemical system & model	Engineering / applied use
	inter-conversion network (HOCl, OCl-, ClO2, ClO2-, ClO3-) with NOM terms, pH-fixed. *Workbook note: from Rougé, Lee, von Gunten & Allard, "Kinetic and mechanistic understanding of chlorite oxidation during chlorination...," Water Research 220 (2022) 118515.*	disinfection — regulatory-compliance and disinfectant-dosing engineering.
`Water Purification_phenol oxidation.xlsm`	Phenol oxidation in water using USER-defined photolysis/oxidant rate laws spanning HSO5-, S2O8--, H2O2, HOCl, OCl-, HOBr competing for UV photons. *Workbook note: from Huang & Zhang, "A comprehensive kinetic model for phenol oxidation in seven advanced oxidation processes...," Water Research X 14 (2022) 100129.*	Models competitive-oxidant phenol destruction under UV — process optimization for oxidant selection in contaminated-water remediation.
`zhang_aerobic-Fitting_Multiple_Datasets.xlsm`	Surface-bound Fe(III)/Fe(II) + ascorbate redox cycling under aerobic conditions with O2, fitted across six datasets.	Iron redox cycling at mineral/water interfaces with oxygen — relevant to iron-mediated contaminant transformation and natural attenuation in aerobic waters/sediments.
`zhang_anoxic-Fitting_Multiple_Datasets.xlsm`	The anoxic counterpart: surface Fe(III)/Fe(II)/ascorbate redox cycling without oxygen, multi-dataset fit.	Anoxic iron redox kinetics for groundwater/sediment geochemistry and contaminant fate under oxygen-limited conditions.

3. Nonlinear, Oscillating & Stereoselective Reaction Engineering

5 workbooks in this group.

Workbook	Chemical system & model	Engineering / applied use
`Oregonator_in_CSTR.xlsm`	Modified Oregonator model of the Belousov-Zhabotinsky oscillating reaction with explicit flow through a CSTR (residence time set on every species).	Textbook nonlinear reaction-engineering case: oscillations, limit cycles and multiplicity in a continuous stirred-tank reactor — used to study reactor stability and dynamic control.
`Pires and Faria Inorg Chem 2021 photochemical chlorate-iodide clock reaction.xlsm`	Detailed chlorate-iodide photochemical clock-reaction mechanism (Pires & Faria, Inorg. Chem. 2021): iodine/chlorine oxy-species autocatalytic network. *Workbook note: from Pires & Faria, "The Photochemical Chlorate–Iodide Clock Reaction," Inorg. Chem. 61(2) 2022, 1178-1187.*	Models clock/autocatalytic kinetics and induction-time control — reaction-engineering insight into autocatalysis and feedback that also underlies halogen water chemistry.
`Chemnet_Pires and Faria Inorg Chem 2021 photochemical chlorate-iodide clock reaction.xlsm`	The Pires & Faria chlorate-iodide photochemical clock mechanism configured to export a reaction network (chemnet/specnet, plus dot/circo graph layouts) for visualization. *Workbook note: network-graph (chemnet) version of the Pires & Faria chlorate-iodide clock model (Inorg. Chem. 2022); O_-prefixed sheets are written out as tab-delimited text on Run.*	The network-graph version of the chlorate-iodide clock model: used to visualize and audit the autocatalytic halogen reaction pathways behind the clock behaviour.
`chlorate_iodine_JACS_FIG_1a.xlsm`	Chlorate + iodide autocatalytic clock mechanism reproducing Figure 1a of the source JACS study (HOI/HIO2/I2/ClO2 network). *Workbook note: the Chlorate-Iodine clock reaction of Oliveira & Faria (JACS 2005, 127, 18022); this run replicates Figure 1a.*	Reproduces a published clock-reaction figure; a validation/benchmark case for autocatalytic halogen kinetics modelling.
`chiral_kinetic_resolution.xlsm`	Dynamic kinetic resolution of chirally labile enantiomers (Noyori BINAP-Ru hydrogenation, Kitamura et al.	Quantifies enantioselectivity vs substrate racemization rates — pharmaceutical/fine-chemical asymmetric-catalysis reactor design and optimization of ee.

Workbook	Chemical system & model	Engineering / applied use
	JACS 1993): competing R/S substrate interconversion and stereoselective product formation.	

4. Enzyme & Biochemical Reaction Engineering

15 workbooks in this group.

Workbook	Chemical system & model	Engineering / applied use
`Chemnet_Enzyme_Inhibition_Model.xlsm`	Non-competitive enzyme inhibition mechanism (E, S, ES, I, EI, EIS, P) with network-export (chemnet/specnet) sheets for reaction-graph visualization.	Bioreactor/biocatalysis kinetics with inhibition; the network export helps visualize and communicate enzyme-mechanism pathways for process and pharmacology work.
`Enzyme_Cluster_Analysis.xls`	The non-competitive enzyme inhibition mechanism used as input to Kintecus's clustering-analysis feature (-cluster switch) with a simple Euclidean-distance similarity matrix. *Workbook note: demonstrates the clustering-analysis feature in Kintecus V3.9 (-cluster switch) using a simple Euclidean-distance similarity matrix.*	Shows clustering of reacting species by trajectory similarity (Euclidean metric) — used to find groups of kinetically similar species in a biochemical network.
`Enzyme_Cluster_Analysis_2.xls`	The same enzyme inhibition mechanism run through Kintecus clustering analysis but using a correlation similarity matrix. *Workbook note: the same clustering-analysis feature using a correlation similarity matrix instead of Euclidean distance.*	Companion clustering-analysis case contrasting the correlation metric with the Euclidean metric for grouping kinetically similar species.
`Enzyme_Regression_Fitting.xlsm`	The core non-competitive-inhibition	Demonstrates fitting enzyme rate constants to a progress curve — the foundational

Workbook	Chemical system & model	Engineering / applied use
	enzyme model with unknown rate constants flagged ('1?') for regression against FDATA/FITPLOT data. *Workbook note: baseline single-dataset rate-constant regression example (FDATA/FITPLOT).*	parameter-estimation workflow for biocatalytic process kinetics.
`Enzyme_Regression_Fitting_BOOTSTRAPPING.xlsm`	Same enzyme fit using bootstrap resampling and thermodynamic linkage (k expressed via 1/Keq) to estimate parameter confidence. *Workbook note: demonstrates the BOOTSTRAP method for accurate standard errors of the fitted parameters.*	Provides statistically rigorous confidence intervals on enzyme kinetic parameters — important for defensible bioprocess design.
`Enzyme_Regression_Fitting_Constraints_fit5.xlsm`	Enzyme fit with explicit bound constraints on rate constants (e.g. 1e3<k<1e9). *Workbook note: shows rate-constant constraints (model worksheet) with the newer -FIT:5 optimizer.*	Shows constrained parameter estimation that keeps fitted enzyme constants physically realistic — a practical regression technique.
`Enzyme_Regression_Fitting_Multi_Absorb.xlsm`	Enzyme fit against multiple absorbance signals (multi-wavelength spectroscopic data, fitdata + fitdata2). *Workbook note: builds special outputs that are functions of concentrations/temperature (here four overlapping absorbance wavelengths) to regress against data*	Fits kinetics to spectrophotometric data where several species absorb — typical of UV-Vis enzyme assays in bioanalytical engineering.

Workbook	Chemical system & model	Engineering / applied use
	when species absorbances overlap.	
`Enzyme_Regression_Fitting_Multiple_Datasets.xlsm`	Enzyme model fitted simultaneously to three experimental datasets (d1/d2/d3, multi-plot). *Workbook note: multi-dataset fit of rate constants across three datasets at the same initial conditions.*	Global fitting across experiments for one consistent enzyme parameter set — best practice for robust biocatalytic kinetic models.
`Enzyme_Regression_Fitting_Multiple_Datasets_and_initial_conditions.xlsm`	Multi-dataset enzyme fit that also varies initial conditions per dataset (O_initial_conditions.txt). *Workbook note: multi-dataset fit of rate constants where each dataset uses different initial conditions.*	Handles experiments run at different starting concentrations in a single global fit — realistic for enzyme assay series at varied substrate loadings.
`Enzyme_Regression_Fitting_WEIGHTS_TEST.xlsm`	Enzyme regression demonstrating data weighting in the objective function. *Workbook note: demonstrates per-point data weighting in the fitdata file via values in parentheses, e.g. 2e-5(0.1).*	Shows how measurement weighting (by uncertainty) affects fitted enzyme parameters — sound statistical practice in kinetic estimation.
`Enzyme_Regression_Fitting_reverse_rate_fit.xlsm`	Enzyme fit where reverse rate constants are tied to forward ones through equilibrium constants (k_rev = k_fwd / Keq). *Workbook note: constrains reverse constants kb to forward constants via the equilibrium constant (reducing 9 parameters to 5); use -FITSTAT:BOOT for errors.*	Enforces thermodynamic consistency between forward/reverse steps while fitting — prevents physically impossible kinetics in reversible enzyme mechanisms.

Workbook	Chemical system & model	Engineering / applied use
`Enzyme_Regression_Fitting_reverse_rate_fit_new_way.xlsm`	Updated approach to the reverse-rate linkage using an explicit fit-links file (O_fit_links.txt) referencing reaction numbers. *Workbook note: the same forward/reverse linkage done through the fit_links mechanism (O_fit_links.txt).*	A cleaner parameter-linking method for thermodynamically consistent reversible enzyme kinetics.
`Enzyme_Regression_Molar_Extinct.xlsm`	Enzyme fit that simultaneously regresses molar extinction coefficients alongside rate constants. *Workbook note: uses -FITWEIGHT:column#:guess to fit a molar extinction coefficient (Kintecus returns 1/epsilon) together with one rate constant.*	Couples spectroscopic calibration (extinction coefficients) with kinetic fitting — needed when absorbance must be converted to concentration during the fit.
`Enzyme_Uncertainty_Analysis.xlsm`	Enzyme model with input uncertainty assigned to rate constants and initial concentrations (e.g. value(.2/1)? notation) for error propagation. *Workbook note: -CONF switch runs 100 kinetic runs with 2-4% Gaussian deviations; model/species cells override values via the number(stddev/1)? notation.*	Propagates kinetic and concentration uncertainty into predicted enzyme behaviour — quantitative risk assessment for bioprocess predictions.
`Enzyme_scanning.xlsm`	Enzyme model scanning a parameter (e.g. substrate from 0.01 to 0.10 M) with 23 stored CONC result sheets and a SCANPLOT.	Generates a family of progress curves vs substrate loading — e.g. building a rate-vs-[S] saturation profile for Michaelis-Menten/inhibition characterization.

Workbook	Chemical system & model	Engineering / applied use
	Workbook note: uses the scan switch to generate a family of runs.	

5. Polymer Reaction Engineering

2 workbooks in this group.

Workbook	Chemical system & model	Engineering / applied use
`POLYMER_MULTIFIT_MULTICONDITIONS.xls`	Free-radical MMA polymerization mechanism (initiation, propagation, termination by combination/disproportionation, chain transfer, inhibition) fitted across three conditions with external condition file. *Workbook note: multi-dataset rate-constant fit at three temperatures (300/325/350 K); initial conditions per dataset set in O_polymer_conditions.txt.*	Models methyl-methacrylate radical polymerization and fits kinetics across multiple operating conditions — core polymer-reactor design and process-development kinetics.
`POLYMER_MW_DISTRIBUTION_CALC.xlsm`	The MMA polymerization mechanism with a dedicated molecular-weight-distribution calculation sheet.	Computes polymer molecular-weight distribution / dispersity from the kinetic run — directly tied to product-quality control in polymer manufacturing.

6. Thermodynamic & Phase Equilibrium

3 workbooks in this group.

Workbook	Chemical system & model	Engineering / applied use
`H2SO4_Equilibrium_Phase.xlsm`	Equilibrium (eqtherm) calculation of the H2SO4(l)/SO2/SO3 system with a concentration-vs-temperature plot.	Predicts sulfuric-acid/SOx equilibrium speciation vs temperature — relevant to contact-process sulfuric-acid plants and SOx handling.
`H2_O2_Equil_Phases.xlsm`	Multi-phase equilibrium of the H2/O2/H2O system (eqtherm) with concentration-vs-temperature output.	Gibbs-energy-minimization style equilibrium of water formation/dissociation vs temperature — combustion-product and steam-system thermodynamics.
`H2_O2_N2_Equilibrium.xlsm`	Equilibrium composition of the H2/O2/N2 system including N-containing species (eqtherm).	Equilibrium NOx and combustion-product prediction in air — adiabatic-flame/equilibrium analysis for emissions and thermodynamic limits.

7. Templates, Tooling, Validation & Teaching Models

13 workbooks in this group.

Workbook	Chemical system & model	Engineering / applied use
`Kintecus_workbook.xls`	The blank master Kintecus workbook (empty model/species with full CONTROL, PARM, therm, fitdata sheets and embedded help).	The starting template for building any new kinetic simulation — the blank reactor 'form' an engineer copies and fills in.
`Kintecus_graphs_templates.xls`	Pre-built graphing templates (CONC and CONCeq plot sheets) for visualizing kinetic and equilibrium output. *Workbook note: graph templates copied into a workbook via right-click > Move or Copy; Kintecus recognizes "ctemplate" (concentration plots) and "ttemplate" (temperature plots).*	Reusable plotting layouts for presenting concentration-time and equilibrium results — reporting/visualization aid.
`Kintecus_10_products_test.xlsm`	A stress/validation case with one reaction producing many products with non-integer stoichiometry (A+B+C ==> D+E+F+2G+3.566H+...).	Verification model checking that the solver handles many products and fractional stoichiometric coefficients correctly — software QA.
`Kintecus_MCM_examples.xls`	Examples of special rate-law directives (TDBR, MTD, MCM, CHEB third-body/temperature-pressure forms) drawn from the Master Chemical Mechanism conventions. *Workbook note: examples of the special MCM/TDBR/MTD/CHEB third-body and temperature/pressure rate directives.*	Reference for encoding complex pressure/temperature-dependent and Master-Chemical-Mechanism rate expressions — used in atmospheric/tropospheric chemistry modelling.
`MCM import macro_v0.4.1_beta.xlsm`	A VBA macro tool that imports Master Chemical Mechanism (MCM) reaction sets and translates their rate expressions into Kintecus format. *Workbook note: macro to import an MCM model from a spreadsheet.*	Automation/tooling that ingests large published atmospheric mechanisms — a productivity utility for air-quality and tropospheric-chemistry modelling.

Workbook	Chemical system & model	Engineering / applied use
`Kintecus_multiwell_cheb_tests.xls`	Test workbook for Chebyshev (CHEB) pressure/temperature-dependent rate representations (multiwell rate surfaces) with SYSOUT. *Workbook note: Kintecus V5.5+ supports Chebyshev expansions (Venkatesh) for pressure falloff and T-dependent rates of multiple-well reactions via the CHEB keyword and a chebdata.txt file.*	Validates Chebyshev-polynomial rate handling used for complex falloff/multiwell reactions — important for accurate pressure-dependent combustion/atmospheric kinetics.
`Chemnet_Simple_Mechanism_Validations.xlsm`	Simple A/B/C interconversion mechanisms implementing the validation cases of Stanbury & Hoffman (2019) with network export.	Teaching/validation set illustrating thermodynamically legal vs illegal mechanism cycles — trains correct mechanism construction and detailed-balance checking.
`Chemnet_Visualize_mechanism_validation_1.xlsm`	Iodate/iodide (Dushman-type) mechanism set up to export a reaction network (chemnet/specnet) for graphical visualization.	Demonstrates turning a kinetic mechanism into a species/reaction graph — a communication and mechanism-auditing aid.
`ChemNet_Combustion_workbook_OH.xlsm`	The H2/O2 OH combustion mechanism configured to export chemnet/specnet reaction-network files.	Shows reaction-flux/network visualization applied to a combustion mechanism — pedagogical and diagnostic for pathway analysis.
`Disease_spread_Endemic.xlsm`	An SI-type epidemiological model (Healthy/Infected/Dead with births) cast as chemical reactions reaching an endemic steady state.	Pedagogical use of chemical-kinetics machinery for population/epidemic dynamics — illustrates that mass-action ODE solvers apply to any rate process, including endemic-equilibrium analysis.
`Disease_spread_Epidemic.xlsm`	An SIR-type model (Healthy/Infected/Recovered/Dead) as reactions producing an epidemic peak-and-decay curve.	Teaching example mapping epidemic outbreak dynamics onto chemical rate equations — analogy for autocatalytic/chain processes.
`Disease_spread_Epidemic_error_analysis.xlsm`	The SIR epidemic model with uncertainty on initial populations and confidence-band output (CONCMIN/MAX/AVG/STD).	Combines the epidemic analogy with Monte-Carlo uncertainty propagation — teaches both dynamic modelling and error analysis.

Workbook	Chemical system & model	Engineering / applied use
`AstroBiology_Ross.xlsm`	A stepwise oligomerization/polymerization network (A1+A1->A2, A2+A1->A3, ...) with paired forward/reverse rates and thermodynamic (delta-G/Keq) annotations, modelling prebiotic chain growth. *Workbook note: from Ross & Deamer, "Prebiotic Oligomer Assembly: What Was the Energy Source?", Astrobiology 19(4), 2019.*	Physical-chemistry/astrobiology model of abiotic monomer-to-polymer assembly — illustrates sequential equilibrium polymerization and free-energy-controlled chain growth.