Kinetic

1- Adsorption kinetic models: Physical meanings, applications, and solving methods

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Abstract

Adsorption technology has been widely applied in water and wastewater treatment, due to its low cost and high efficiency. The adsorption kinetic models have been used to evaluate the performance of the adsorbent and to investigate the adsorption mass transfer mechanisms. However, the physical meanings and the solving methods of the kinetic models have not been well established. The proper interpretation of the physical meanings and the standard solving methods for the adsorption kinetic models are very important for the applications of the kinetic models. This paper mainly focused on the physical meanings, applications, as well as the solving methods of 16 adsorption kinetic models. Firstly, the mathematical derivations, physical meanings and applications of the adsorption reaction models, the empirical models, the diffusion models, and the models for adsorption onto active sites were analyzed and discussed in detail. Secondly, the model validity evaluation equations were summarized based on literature. Thirdly, a convenient user interface (UI) for solving the kinetic models was developed based on Excel software and provided in supplementary information, which is helpful for readers to simulate the adsorption kinetic process.

Keywords

Author Keywords
AdsorptionKinetic modelPhysical meaningSolving method
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SURFACE-DIFFUSION MODELAQUEOUS-SOLUTIONACTIVATED CARBONMASS-TRANSFERWASTE-WATERLANGMUIR KINETICSHEAVY-METALSPHOSPHATE ADSORPTIONNONLINEAR-REGRESSIONELOVICH EQUATION

Kinetic

2- Manufacturing Process Development for Belzutifan, Part 5: A Streamlined Fluorination-Dynamic Kinetic Resolution Process

By:
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Abstract

Here we report the fluorination-dynamic kinetic resolution (DKR) process for the commercial supply of belzutifan (MK-6482). Key process safety and robustness issues in the Selectfluor fluorination reaction were identified and addressed on the basis of increased mechanistic understanding. Aggressive process optimization enabled a single-pot direct isolation process that allowed delivery of the fluorodiol product with low process mass intensity.

Keywords
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fluorinationdynamic kinetic resolutionDKRNoyori asymmetric reductionsingle-pot direct isolationthrough process
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3- Microbiological predictive modeling and risk analysis based on the one-step kinetic integrated Wiener process

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Abstract

The actual growth-monitoring data of microbial hazards in food are characterized by uncertainty, accumulation, discreteness, and nonlinearity, and thus it is difficult to accurately predict and analyze food safety microbio-logical risks in real time. Hence, we propose an approach of microbiological predictive modeling and risk analysis based on the one-step kinetic integrated Wiener process (OS-WP). First, the microbial tertiary prediction model was directly constructed through one-step kinetic analysis. Then, the WP was integrated with a tertiary model for predictive modeling of the actual microbial stochastic growth. Second, an indicator, "remaining safety life" (RSL), was introduced to analyze the potential microbiological risk on the basis of the established prediction models. Finally, the maximum likelihood estimation was used obtaining the model parameters online, and for calculating the RSL value in real time. The OS-WP approach was applied to a case study of the mixed mildew hazard during wheat storage. For different datasets, the root mean square error (RMSE) of the microbiological predictive model was less than 1.5; the relative RMSE of the RSL prediction reached 6.77%; the running time was less than 0.6 s. The result showed that the proposed approach is effective and feasible in modeling the actual growth of microbial hazards in food and can achieve online risk analysis. It can provide valuable microbiological early warning information to risk-management and decision-making departments for ensuring food safety.

Keywords
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Food safetyMicrobiological predictive modelingRisk analysisOne-step kinetic analysisWiener process

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FOOD SAFETYPARAMETER-ESTIMATIONCOMPUTER-SIMULATIONASPERGILLUS-FLAVUSGROWTHIDENTIFICATIONSYSTEMSTEMPERATUREMICROORGANISMSSURVIVAL

4- A Theoretical Framework for Ratiometric Single Ion Luminescent Thermometers-Thermodynamic and Kinetic Guidelines for Optimized Performance

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Abstract

Luminescence (nano)thermometry is an increasingly important field for remote temperature sensing with high spatial resolution. Most typically, ratiometric sensing of the luminescence emission intensities of two thermally coupled emissive states based on a Boltzmann equilibrium is used to detect the local temperature. Dependent on the temperature range and preferred spectral window, various choices for potential candidates appear possible. Despite extensive experimental research in the field, a universal theory covering the basics of luminescence thermometry is virtually nonexistent. In this manuscript, a general theoretical framework of single ion luminescent thermometers is presented that offers simple, user-friendly guidelines for both the choice of an appropriate emitter and respective embedding host material for optimum temperature sensing. The results show that the optimum performance (thermal response and sensitivity) aroundT(0)is realized for an energy gap increment E(21)between thermally coupled levels between 2k(B)T(0)and 3.41k(B)T(0). Analysis of the temperature-dependent excited state kinetics shows that host lattices in which increment E(21)can be bridged by one or two phonons are preferred over hosts in which higher order phonon processes are required. Such a framework is relevant

for both a fundamental understanding of luminescent thermometers but also the targeted design of novel and superior luminescent (nano)thermometers.

Keywords
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Boltzmann distributionexcited state dynamicsluminescence thermometry

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