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材料化学工程与纳米技术

塑料食品包装材料化学物迁移的数值模拟

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摘要

基于有限差分方法数值模拟了塑料食品包装材料化学物向食品（模拟物）的迁移及迁移物在食品内的不稳定性。结果表明，扩散系数DP决定了迁移的动力学过程，分配系数KP,F表征平衡时化学物在包装材料和食品内的浓度比值，平衡时食品内的化学物浓度随化学物在包装材料内的初始浓度Cin的增加而增加。对于多层复合包装，阻隔层可显著减缓污染物层内化学物向食品的迁移，从而达到保证食品安全的目的，阻隔层厚度LR影响阻隔功效。化学迁移物在食品内存在不稳定现象，这将导致实验结果低估其向食品的迁移。

关键词

化学物迁移 数值模拟 塑料包装 食品包装安全 不稳定性

分类号

Numerical simulation of migration of chemical substances from plastic food packaging materials into foods

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Abstract

The US Food and Drug Administration (FDA) and European Commission (EC) have carried out theoretical and experimental researches on migration of chemical substances.Migration of chemical substances from plastic packaging materials into foods contaminates foods and finally endangers people’s health, and has been widely studied and discussed.Numerical simulation of migration of chemical substances (migrants) from plastic food packaging materials into foods and the instability of migrants in foods were performed by using the finite difference method (FDM).The results showed that the diffusivity of migrants DP was key to migration dynamics.Partition coefficient KP,F represents the ratio of migrant concentration in packaging materials to that in foods at equilibrium.The concentration of migrants in foods at equilibrium increased with the increase of its initial concentration in packaging materials.For multilayer packaging, functional barrier layer was able to efficiently delay migration and assure food safety.The thickness of barrier layers influenced the barrier effect and then the ability to protect foods from contamination.The instability of migrants in foods is a problem newly found and leads to underestimation of migration.

Key words

migration of chemical substances numerical simulation plastic packaging food packaging safety instability

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