



Adsorptive transformation of heat: Principles of construction of adsorbents database

Yuriy I. Aristov

Boreskov Institute of Catalysis, 5 Ak. Lavrentieva St., Novosibirsk 630090, Russia

ARTICLE INFO

Article history:

Received 1 August 2010

Accepted 14 February 2011

Available online 26 February 2011

Keywords:

Adsorptive heat transformer

Adsorption equilibrium

Adsorbents database

ABSTRACT

Developing a database of adsorbents promising for adsorptive transformation of heat is very timely. This database would play an important role in unification of adsorbent properties, correct comparison of various adsorbents, theoretical analysis, mathematical modeling and brief estimation of heat transformation cycle performance. In this paper, we discuss principles of creating such database, consider the adsorbent properties which should be given there, and address the issues of their measurement and calculation. A tentative list of common and innovative adsorbents to be presented in the database is discussed as well.

© 2011 Elsevier Ltd. All rights reserved.

1. Introduction

An adsorbent is a key element of an adsorptive heat transformer, AHT (heat pump, chiller, amplifier), and harmonization of the adsorbent with the cycle is of prime importance. It is traditionally reached by **screening** of known adsorbents to select the best one for a given cycle. “Old” working pairs “adsorptive–adsorbent” that are principal for AHT applications were selected in the last century by [1]. An alternative way is **tailoring** of novel adsorbents adapted to this cycle [2]. The main idea of the latter approach is that for each particular adsorptive cycle there is an optimal adsorbent, the thermodynamic characteristics of which could allow perfect performance of this cycle. The first step of the analysis is the formulation of requirements of this desirable (ideal) adsorbent. The final step is to design and synthesize a new adsorbent with sorption properties close or even equal to those determined before as perfectly fitting the cycle. Thermodynamic requirements of an optimal adsorbent were first considered for a basic AHT cycle in [3] and completed in [2]. This analysis showed that the optimal adsorbents for various AHT applications can significantly differ. Besides, quite different adsorbents are needed for the same AHT application in different climatic zones [2]. Thus, the appearance of many new adsorbents adapted to particular boundary conditions of AHT cycle can be forecasted. Indeed, several innovative materials have recently been synthesized and considered for AHT applications, namely, composites “salt in porous matrix” [4,5], metal–aluminophosphates [6,7], metal–organic frameworks [2,8], etc., and a number of data on adsorption properties of “old” and “new” materials are booming.

E-mail address: aristov@catalysis.ru.

Hence, it is well timed to systematize and tabulate adsorption properties of promising materials to make them available to anyone. Such a database would be very useful for unification of adsorbent properties, correct comparison of various adsorbents, theoretical analysis, mathematical modeling and brief estimation of AHT cycle performance. In this paper, we discuss possible approaches to creating such database, consider the adsorbent properties which should be presented there, and address the issues of their measurement and/or calculation. Finally, a tentative list of “old” and “new” adsorbents to be included in this database is discussed.

2. Principles of the database construction

The AHT performance essentially depends on both *thermodynamic* and *dynamic* properties of the working pair “adsorptive–adsorbent”. Thus, every thermodynamic or dynamic property of usable adsorbents which is essential for analyzing (modeling) AHT cycles should be presented in the database. We adopt in this paper definitions recommended by IUPAC [9], e.g. “the material in the adsorbed state is known as the *adsorbate*, as distinct from the *adsorptive*, i.e. the substance in the fluid phase which is capable of being adsorbed”.

2.1. Thermodynamic data

For plotting an AHT cycle and analyzing its thermodynamic performance one needs to know data on adsorption (desorption) equilibrium in the system “sorptive–sorber”, the isosteric heat of sorption Q_{is} and the specific heat capacity of adsorbent $C_p(w, T)$ at various adsorbate uptakes w and temperatures T .