Thermodynamic Limits for Dehalogenation of Producer Gas by Na2CO3, NaAlO2, CaO/CaCO3, BaO/BaCO3 and Mixed CaO-BaO/BaCO3 Sorbents.

Svoboda, Karel
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[1]K. Svoboda, [2]J. Leitner, [1]J. Havlica, [1,3]J. Brynda, [3]S. Skoblia, [1]M. Hartman, [1]M. Pohořelý, [4]H.-T. Hsu
[1]Institute of chemical process fundamentals of the CAS, v.v.i., Rozvojová 135, 165 02 Praha 6, CZ, E-mail: svoboda@icpf.cas.cz Tel. + 420 220 390 160 Fax: +420 220 920 661
[2]Dep. of Solid State Engineering, Faculty of Chemical Technology, University of Chemistry and Technology Prague, Technická 3, 166 28 Prague 6, CZ, E-mail: jindrich.leitner@vscht.cz
[3]Department of Gas, Coke and Air Protection, University of Chemistry and Technology Prague, Technická 5, 166 28 Prague 6, CZ, E-mail: Sergej.Skoblja@vscht.cz
[4]Chemistry Division, Institute of Nuclear Energy Research, No. 1000, Wenhua Rd., Jiaan Village, Longtan Township, Taoyuan County 32546, Taiwan (R.O.C.)
E-mail: dukeininer@iner.gov.tw Tel.: 886-3-4711400 ext. 5346

The advanced applications (e.g. catalytic processes and fueling of high temperature fuel cells) of producer gas from gasification processes are extremely sensitive to inorganic and organic contaminants in the gas and on limits of cleaning processes. Among the gas contaminants, stable halogen containing compounds, HCl, HF and HBr produced in the gasification process should be considered as clear candidates for deep removal. Producer gas cleaning for attaining hydrogen-halides concentrations approx. below 1 ppm_v requires either application of low temperature wet absorption processes or, particularly for fueling of high temperature fuel cells (SOFC), deployment of medium and high temperature (600 – 1200 K) cleaning methods with solid sorbents. Our study is focused on thermodynamic analyses and minimization of Gibbs energy for gas de-halogenation (removal of HCl, HF and HBr) by selected solid sorbents (Na_2CO_3, $NaAlO_2$, $CaO/CaCO_3$, $BaO/BaCO_3$, and mixtures containing $CaO\text{-}BaO/BaCO_3$). The cheap Na_2CO_3 and $NaAlO_2$ based sorbents are suitable for deep removal of HCl and particularly HBr at temperatures below 800 K, but they are less suitable for HF removal. For attaining low HF equilibrium concentrations rather the $CaO/CaCO_3$ based sorbents are the best choice. The promising $BaO/BaCO_3$ based sorbents and mixed CaO-BaO/BaCO3 sorbents for removal of HCl, HBr and HF (or even their mixtures with H_2S) are dependent on appropriate solid solution form stabilizing BaO for its sorption applications, because BaO has significantly more favorable equilibria than $BaCO_3$ with all studied hydrogen-halides. Unfortunately stabilization of BaO in mixtures with CaO and similar compounds requires temperatures over 1150 K – 1200 K.