Available online at www.sciencedirect.com

ScienceDirect

Applied Energy 84 (2007) 853–862

APPLIED ENERGY

www.elsevier.com/locate/apenergy

Analysis of energy use and carbon losses in the chemical industry

Maarten Neelis [a,*], Martin Patel [a], Pieter Bach [b], Kornelis Blok [a]

[a] *Utrecht University, Copernicus Institute, Department of Science, Technology and Society, Heidelberglaan 2, 3584 CS Utrecht, The Netherlands*

[b] *Energy Research Centre of The Netherlands, Unit Energy Efficiency in Industry, Westerduinweg 3, 1755 LE Petten, The Netherlands*

Available online 26 March 2007

Abstract

A preliminary bottom-up analysis of the energy use in the chemical industry has been performed, using a model containing datasets on production processes for 52 of the most important bulk chemicals as well as production volumes for these chemicals. The processes analysed are shown to cover between 70% and 100% of the total energy use in the chemical sector. Energy use and the heat effects of the reactions taking place are separately quantified. The processes are also compared with energetically-ideal processes following the stoichiometric reactions. The comparison shows that there is significant room for process improvements, both in the direction of more selective processes and in the direction of further energy-savings.

Keywords: Chemical industry; Energy use; CO_2 emissions; Energy efficiency; Selectivity

1. Introduction and purpose

Numerous studies describing the structure of energy use in the chemical industry are available from the open literature. Some studies aim to determine life-cycle energy-use and CO_2 emission data for intermediates and plastics [1–3], while other studies aim to give an overview of the chemical sector for a given region [4–7]. Yet other studies aim to

* Corresponding author. Tel.: +31 30 2537600; fax: +31 30 2537601.
E-mail address: m.l.neelis@chem.uu.nl (M. Neelis).

0306-2619/$ - see front matter
doi:10.1016/j.apenergy.2007.01.015

describe Best Available Technologies [8] or to define potentials for process improvement [9–11]. The studies differ widely in geographical scope and in completeness, key assumptions and aggregation level. The underlying data for all the studies are dispersed and it is difficult to use them directly for bottom-up analyses of energy use and CO_2 emissions in the chemical industry for various regional boundaries and for various levels of aggregation. We therefore developed a model, containing a variety of datasets on production processes for 52 of the most important bulk chemicals in terms of production volume. The model also contains production volumes for those chemicals and shares of individual process routes in three geographical regions: The Netherlands, Western Europe[1] and the World. The model facilitates making detailed bottom-up analyses of energy use and CO_2 emissions both at the level of individual processes and at the level of the chemical sector as a whole for the three regions included. In this paper, we give some preliminary results of such an analysis in which we focus on energy use, with minor attention to CO_2 emissions. Questions that will be answered are (a) how is the energy use in the chemical sector distributed over the various processes and especially (b) what are the main components of energy use and CO_2 emission in the chemical industry (e.g. energy use versus reaction losses)?

2. Scope methodology and data sources

The model contains datasets for 73 different production processes[2] for 52 of the most important organic bulk-chemicals[3] in terms of production volume. For each of those chemicals, we included:

- The production volume in The Netherlands, Western Europe and the World.
- The share of the various production processes in these three regions, if the chemical can be made via more than one production route.
- The heat and Gibbs free-energy of reaction of the stoichometric reaction, thereby allowing a comparison between the actual process and the ideal process.

For the 73 process routes, a total of 250 datasets is included in the model. The key data as found in the literature are complemented with background data on the carbon content, the calorific value and the price of raw materials, products and energy commodities used. Most datasets were taken from the open literature sources like [12–14], complemented with some confidential datasets available to the authors. The two most important data sources for the production data and for the shares of the various process routes have been [15,16]. In cases where we did not have production data, we used capacity data instead. The most recent production data were used and no production data older than the mid 1990s was used. A major difficulty is the incomparability of the various datasets from the literature. Some sources refer explicitly to current Best Available Technologies, whereas other sources give data for the European average in a given year. For the analyses shown in Section 3 of this paper, we have chosen the dataset, which most likely represents the average

[1] Defined as the European Union (15 countries) and Norway and Switzerland.

[2] Some chemicals can be made from various raw materials, which explains the number of process routes to be larger than the number of chemicals.

[3] Complemented with chlorine and ammonia.