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# **Bibliometric Analysis of Thermodynamic Research: A Science Citation Index Expanded-Based Analysis**

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Hui-Zhen Fu and Yuh-Shan Ho

Additional information is available at the end of the chapter

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## **1. Introduction**

Thermodynamics is the study of energy and its transformation (Holman, 1985). This subject has evolved since the beginning of the eighteenth century (Look & Saucer, 1982). Most studies of thermodynamics are primarily concerned with two forms of energy: heat and work (Holman, 1985; Keizer, 1985; Rosakis et al., 2000). Thermodynamics advanced dramatically in the 1960s and 1970s, primarily in the area of critical phenomena (Callen, 1985). In recent years, thermodynamic research has been conducted in more systems, such as corn-ethanol biofuel cycle (Patzek, 2004), lipid-peptide interactions (Seelig, 2004), DNA structural motifs (SantaLucia & Hicks, 2004), and glass-forming substances (Ngai, 2000).

Bibliometrics, as a measure of scientific performance, has been widely applied to research evaluation for a long period (Saracevi & Perk, 1973; Luukkonen, 1990; Friedberg, 2000). It has been employed to evaluate various researches, for example biology (Sainte-Marie 2010), desalination research (Tanaka & Ho, 2011), solid waste research (Fu et al., 2010), acupuncture research (Han & Ho, 2011), and global climate change (Li et al., 2011). In exited bibliometric analyses, the analyzed aspects usually covering languages (Alfaraz & Calvino, 2004; Chiu & Ho, 2007; Ferrara, 2011), annual publication outputs (Chiu & Ho, 2007; Tsay, 2008), journals (Schubert et al., 1989; Tsay, 2008), categories (Moed et al., 1995; Yamazaki, 1994), and contributing countries and institutions (Schubert et al., 1989; Chiu & Ho, 2007; Tanaka & Ho, 2011; Li et al., 2011). In recent years, author keywords which could provide a reasonably detailed picture of the article's subject (Garfield, 1990), have been quantitatively analyzed to figure out the research emphases and trends (Chiu & Ho, 2007; Fu et al., 2010; Li

et al., 2011). To analyze these aspects, the common evaluation indicators number of publications and their publication share were utilized (Schubert et al., 1989; Rehn et al., 2007). Impact factor was introduced by Garfield and Sher (1963) to help select additional source journals using the recent citations received from other journals, and has been also widely used to rank and evaluate journals (Garfield, 1996; Moed, 2002). In particular, the five indicators including total, independent, collaborative, first author, and corresponding author articles have been recently used to compare the publication performance of countries and institutions in the researched of Japanese lung cancer (Ho et al., 2010), solid waste research (Fu et al., 2010), desalination research (Tanaka & Ho, 2011), acupuncture research (Han & Ho, 2011), global climate change (Li et al., 2011), and estuary pollution (Sun et al., 2012). In addition, rankings are useful indicators, especially in terms of institutions and researchers in urgent demand by politics (Weingart, 2003). These indicators including number of publication, publication share, impact factor, rankings, and five newly indicators were utilized for the evaluation of thermodynamics research.

The aim of this study was to systematically evaluate not only the publication characteristics of languages, annual publication outputs, journals and Web of Science categories, and national and inter-institutional contributors, but also the research emphases and trends by author keywords to obtain an overview of thermodynamic research during the period from 1991 to 2010.

## 2. Methodology

### 2.1. Data collection

Documents used in this study were derived from the Science Citation Index Expanded (SCI-Expanded) database of the Web of Science, the Thomson Reuters. According to Journal Citation Reports (JCR), it indexes 8,073 journals with citation references across 174 scientific disciplines in 2010. The data was collected on November 20 in 2011, and the detail data collection process is illustrated in Fig. 1. Firstly, thermodynamics related keywords including “thermodynamic”, “thermodynamics”, “free energy change”, “enthalpy change”, and “entropy change” were searched in terms of topic (including four parts: title, abstract, author keywords, and KeyWords Plus) within the publication year limitation from 1991 to 2010 based on SCI-Expanded. Total 157,140 documents were therefore found out. However, these 157,140 documents contained the documents not closely relating to thermodynamics which was searched only in terms of KeyWords Plus which providing search terms extracted from the titles of papers cited in each new article listed in *Current Contents* (Garfield, 1990). To efficiently obtain the characteristics of thermodynamics, this study only focused on the documents (50,865) with searching keywords in front page which including three parts: title, abstract, and author keywords, while the documents where searching keywords only appeared in KeyWords Plus were excluded. These documents consists of 19 document types, where articles (41,245) dominants with a percentage of 81%, followed by proceedings paper (4,860; 10%), meeting abstract (1,787; 3.5%), and review (1,407; 2.8%).

Finally, the journal articles (41,245) were extracted from the 50,865 documents for subsequent analyses.

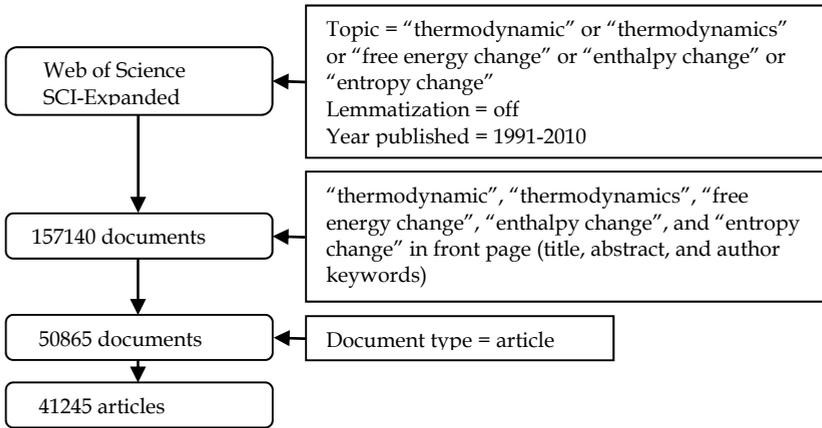


Figure 1. Data collection process for searching thermodynamic related research

### 2.2. Analyzing structure

The analyzing aspects were divided into five sections from different angles. To be specific, the analytic structure of analytic structure of bibliometric analysis of thermodynamic research is presented in Fig. 2. The first section dealt with the basic information covering the distribution of languages and annual production. The second section revealed the performance of productive journals and Web of Science categories. Then national contributors countries and institutional contributors institutions were analyzed in the following third and fourth sections. Finally, recent research emphases and trends were examined by the frequency of author keywords.

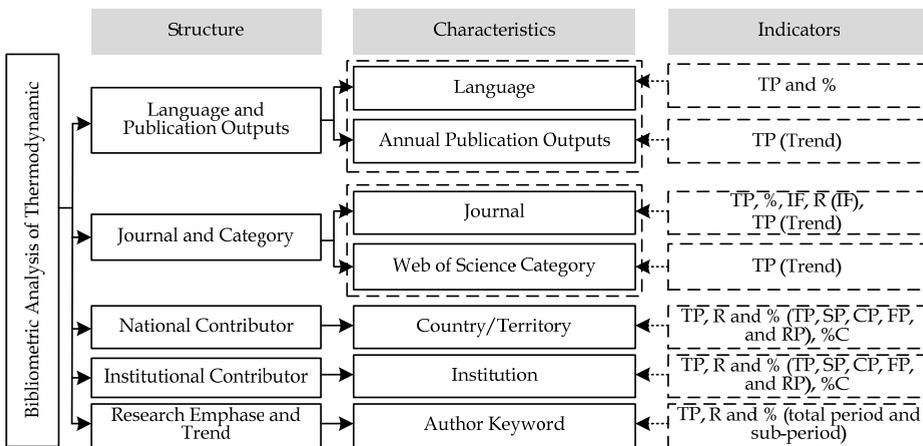


Figure 2. Analytic structure of bibliometric analysis of thermodynamic research

### 2.3. Indicators and acronyms

The indicators displayed in Fig. 2 for detail analysis are explained in Table 1. As for the section of national and institutional contributors, some newly indicators (CP, SP, FP, and RP) were employed to evaluate the performance of countries/territories and institutions. The institutions' and countries/territories' contributions were identified by the appearance of at least one author in the publications. Collaboration type was determined by the addresses of the authors. The articles were classified by four types for country/territory and institution. (1) The term "single country article" was assigned if the researchers' addresses were from the same country. The term "single institution article" was assigned if the researchers' addresses were from the same institution. (2) The term "internationally collaborative article" was designated to those articles that were coauthored by researchers from multiple countries. The term "inter-institutionally collaborative article" was assigned if authors were from different institution. (3) The term "first author article" was assigned if the first author was from the country/territory or institution for analysis. (4) The term "corresponding author article" was assigned if the corresponding author was from the country/territory or institution for analysis. In addition, the acronyms used in the following analysis were listed in Table 2.

Abbreviation	Indicators
TP	Number of scientific publications by the analyzed unit (document type, language, year, journal, Web of Science category, country/territory, institution, or author keyword)
%	Number of papers of an actor (document type, language, journal, country/territory, institution, or author keyword) as a share of the total number of articles
%C	Number of articles of "internationally collaborative articles" or "inter-institutionally collaborative articles" as a share of the number of articles of an actor (country/territory or institution)
IF	Impact factor reported in Journal Citation Reports 2010
SP	Number of "single country articles" or "single institution articles"
CP	Number of "internationally collaborative articles" or "inter-institutionally collaborative articles"
FP	Number of "first author articles"
RP	Number of "corresponding author articles"
R	Rankings of number of articles (TP, SP, CP, RP, or FP) by countries or institutions

**Table 1.** Explanation of the abbreviations used in subsequent analysis

## 3. Results and discussion

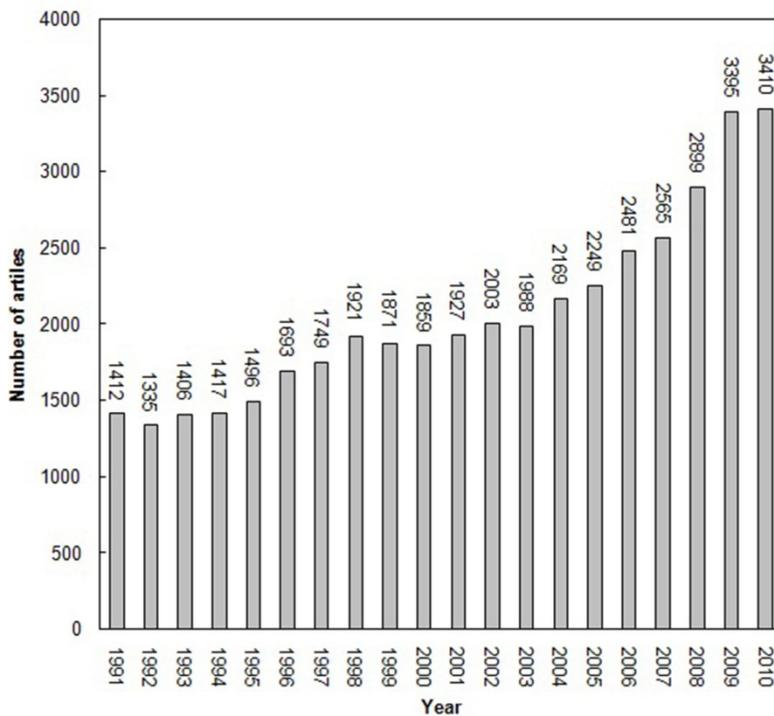
### 3.1. Language and publication outputs

There are 41,245 articles with 17 languages used. English which had 38,976 articles (94%) is the most frequently used language in thermodynamic research. The other languages used in more than 100 articles were Russian (863), Chinese (156), French (151), Japanese (147), and

Full Name	Acronyms
Canada, France, Germany, Italy, Japan, Russia, the UK, and the USA	G8
Canada, France, Germany, Italy, Japan, the UK, and the USA	G7
Chinese Academy of Sciences	CAS
Russian Academy of Sciences	RAS
Central South University	CSU
Naval University of Engineering	NUE
calculation of phase diagram	CALPHAD

**Table 2.** Introduction of the acronyms used in subsequent analysis

German (146). Some other languages that were less used were as follows: Spanish, Portuguese, Polish, Czech, Korean, Ukrainian, Croatian, Hungarian, Slovak, Serbo-Croatian, and Romanian. The high proportion of English also appears in other research areas, such as 94% of desalination research (Tanaka & Ho, 2011), and 93% in acupuncture research (Han & Ho, 2011). Non-English language publications considerably dilute the the measured impact of published articles (van Raan, 2005).



**Figure 3.** The growth trend of articles in thermodynamic research

Journal	TP (%)	IF	Web of Science category (rankings by IF)
Russian Journal of Physical Chemistry A	827 (2.0)	0.503	physical chemistry (114/127)
Journal of Alloys and Compounds	768 (1.9)	2.134	physical chemistry (63/127); multidisciplinary materials science (50/225); metallurgy & metallurgical engineering (5/76)
Physical Review B	741 (1.8)	3.774	condensed matter physics (13/68)
Journal of Chemical Physics	716 (1.7)	2.920	atomic, molecular & chemical physics (7/33)
Journal of Chemical Thermodynamics	697 (1.7)	2.794	thermodynamics (3/51); physical chemistry (46/127)
Thermochimica Acta	652 (1.6)	1.899	analytical chemistry (33/73); physical chemistry (71/127)
Biochemistry	601 (1.5)	3.226	biochemistry & molecular biology (120/286)
Journal of Physical Chemistry B	584 (1.4)	3.603	physical chemistry (32/127)
Fluid Phase Equilibria	483 (1.2)	2.253	thermodynamics (5/51); physical chemistry (61/127); chemical engineering (24/135)
CALPHAD-Computer Coupling of Phase Diagrams and Thermochemistry	450 (1.1)	1.429	thermodynamics (16/51); physical chemistry (81/127)
Physical Review E	444 (1.1)	2.352	fluids & plasmas physics (8/31); mathematical physics (4/54)
Journal of Colloid and Interface Science	411 (1.0)	3.066	physical chemistry (40/127)
Journal of Chemical and Engineering Data	400 (1.0)	2.089	multidisciplinary chemistry (44/147); chemical engineering (28/135)
Surface Science	382 (0.93)	2.010	physical chemistry (69/127); condensed matter physics (19/68)
Journal of Solution Chemistry	360 (0.87)	1.335	physical chemistry (85/127)
Journal of Molecular Biology	339 (0.82)	4.008	biochemistry & molecular biology (86/286)
Journal of the American Chemical Society	317 (0.77)	9.019	multidisciplinary chemistry (11/147)
Physical Review D	278 (0.67)	4.964	astronomy & astrophysics (8/55); particles & fields physics (5/27)
Physical Review Letters	262 (0.64)	7.621	multidisciplinary physics (5/80)

Journal	TP (%)	IF	Web of Science category (rankings by IF)
Langmuir	242 (0.59)	4.268	multidisciplinary chemistry (24/147); physical chemistry (29/127); multidisciplinary materials science (26/225)

**Table 3.** Characteristics of top 20 journals with the most articles in thermodynamics

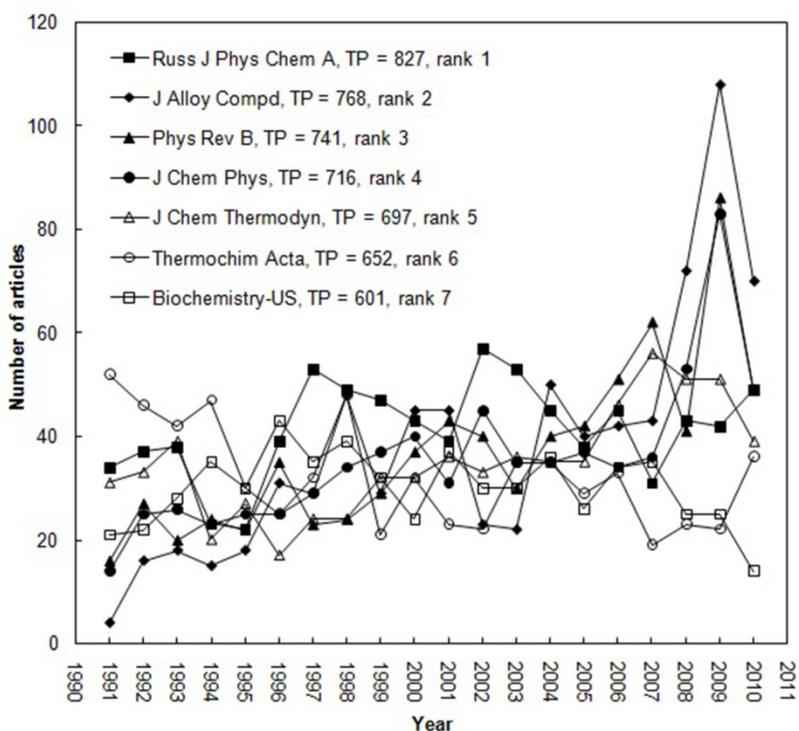
The thermodynamic research revealed a growth trend through the study period, especially in recent years. The number of articles has been climbing up from 1991 to 2010 in Fig. 3. According to the annual growth rate, it can be divided into two stages: 1991-2003 and 2004-2010. In the first stage, the growth rate was 48 articles per year from 1,412 in 1991 to 1,988 in 2003, while in the second stage the growth rate has risen four-fold to 203 articles per year from 2,169 in 2004 to 3,410 in 2010.

## 3.2. Journals and Web of Science categories

### 3.2.1. Journals

The total articles (41,245) were published in 2,434 sources among 150 Web of Science categories. Table 3 lists the top 20 journals with the greatest number of articles. The impact factors of these journals were also exhibited as reputation of a journal attached much attention by the authors and editors (van Raan, 2001). Approximately 24% of the articles resided in these 20 journals. *Russian Journal of Physical Chemistry A* (IF = 0.523) which was founded in 1930, published the most articles (827; 2.0%). Its former was *Zhurnal fizicheskoi khimii* (1930-1999) and *Russian Journal of Physical Chemistry* (1999-2006). Articles published in this journal concern chemical thermodynamics and thermochemistry (<http://www.maik.ru/cgi-perl/journal.pl?name=physcha&page=main>) which is closely related to the topic of this study.

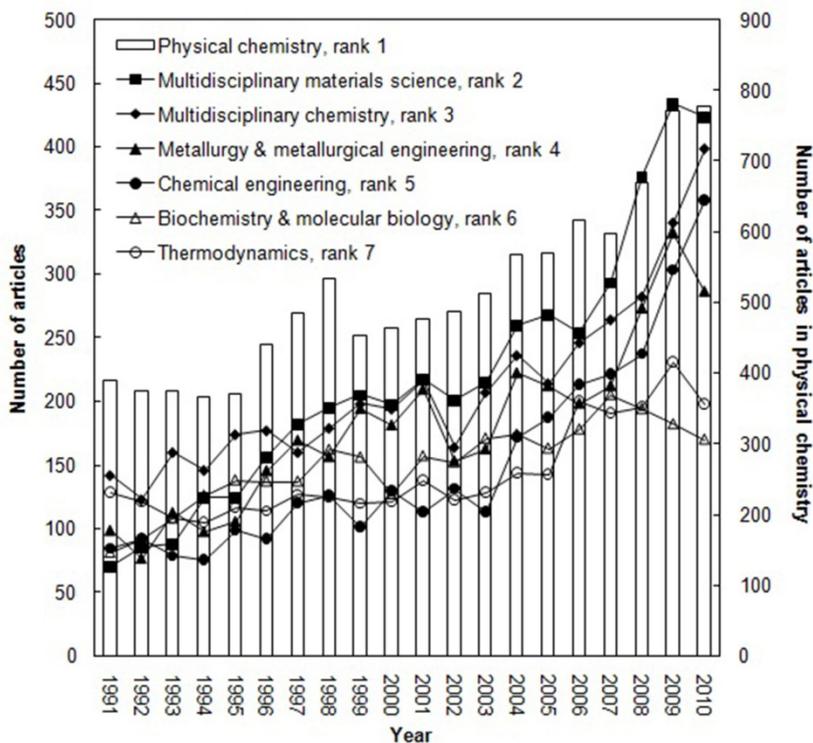
Among the total institutions (1,004) contributing to *Russian Journal of Physical Chemistry A*, 831 institutions (83%) belonged to Russia while only 173 institutions (17%) belonged to other countries. Following three journals: *Journal of Alloys and Compounds* (IF = 2.134), *Physical Review B* (IF = 3.774), and *Journal of Chemical Physics* (IF = 2.920), all had the more than 700 articles. However, the journal which had the highest IF (9.019) was *Journal of the American Chemical Society* in the category of multidisciplinary chemistry which was ranked 17<sup>th</sup>. *Physical Review Letters* in multidisciplinary physics category was ranked 19<sup>th</sup> in the list and ranked 2<sup>nd</sup> in terms of IF (7.621). Furthermore, of these 2,434 sources, 1,828 (75%) sources only contained less than 10 articles; 519 (21%) sources contained 11-100 articles, 60 (2.5%) sources contained 101-200 articles; 20 (0.82%) sources contained 201-600 articles; and seven sources (0.28%) contained more than 600 articles, accounting for 11 percent of the total articles. The trends of the annual publication outputs of the top core seven journals are displayed in Fig. 4. The curves of these seven journals (*Russian Journal of Physical Chemistry A*, *Journal of Alloys and Compounds*, *Physical Review B*, *Journal of Chemical Physics*, *Journal of Chemical Thermodynamics*, and *Thermochimica Acta Biochemistry*) had been interlacing in the study period. However, after 2008, *Journal of Alloys and Compounds* which published 108 articles in 2009 and 70 articles in 2010 showed its domination in the thermodynamic field.



**Figure 4.** The trends of top seven journals with more than 600 articles

### 3.2.2. Web of Science categories

As for category analysis, excluding the 84 articles without subject category information, the remained 41,161 articles were analyzed. The most common category was physical chemistry (10,295; 25%), followed distantly by other categories. A half of the above top 20 journals are assigned to the category of physical chemistry. Within the total 150 Web of Science categories, 92 categories (61%) published articles less than 100 articles; 40 categories (27%) published 101-1000 articles; 12 categories (8.0%) published 1,001-3,000 articles; only six categories (4.0%) published more than 3,000 articles. The six core categories including physical chemistry, multidisciplinary materials science, multidisciplinary chemistry, metallurgy & metallurgical engineering, chemical engineering, and biochemistry & molecular biology, took the majority of the total articles with a great percentage of 55%. As illustrated in Fig. 5, these categories showed greater growth rates in recent years than those in 1990s. These trends were similar to the above trends of annual total publication outputs. The articles of position 1<sup>st</sup> category of physical chemistry which contained 127 journals increased from 390 in 1991 to 777 in 2010. The 2<sup>nd</sup> position category of multidisciplinary materials science which included 225 journals increased six-fold from 70 in 1991 to 423 in 2010.



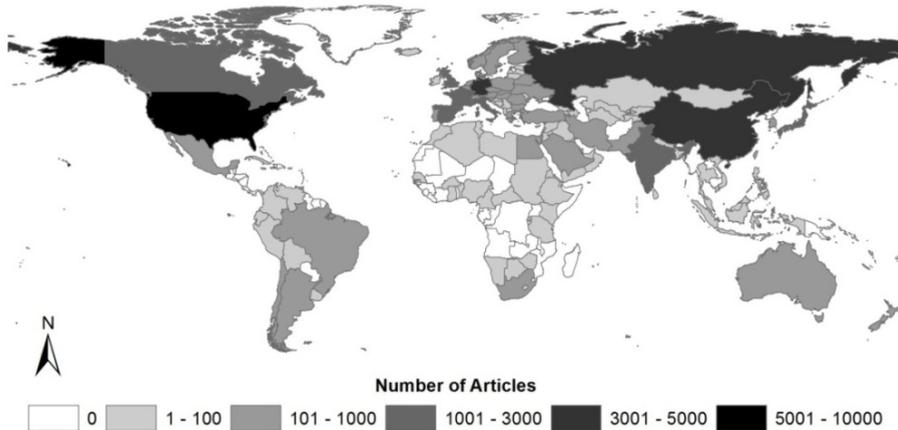
**Figure 5.** The trends of top seven Web of Science categories with more than 3000 articles

### 3.3. National contributors

#### 3.3.1. Global geographical distribution

Excluding 263 articles without any author address information on the Web of Science, the 40,982 articles originated from 128 countries. Articles originating from England, Scotland, Northern Ireland, and Wales were reclassified as being from the United Kingdom (UK) (Chiu & Ho, 2005). Articles from Hong Kong were included in the ones from China. The geographical global distribution of thermodynamic research is shown in Fig. 6. According to their production, the 128 countries were divided into five parts. Particularly, 81 countries (63%) belonged to the first part of 1-100 articles; 36 countries (28%) belonged to the second part of 101-1,000 articles; seven countries (Japan, France, India, Italy, UK, Spain, and Canada) belonged to the third part of 1,001-3,000 articles; three countries (China, Russia, and Germany) belonged to the fourth part of 3,001-5,000 articles; and only one country (USA) which totally published 9,161 articles, belonged to the fifth part of 5,001-10,000 articles. Although there were only 11 countries which published more than 1,000 articles, these 11 countries produced 77% articles. The majority of articles originated from a small number of particular countries. Furthermore, five continents contributed to the thermodynamics

research differently. Europe with 42 countries published the most articles 22,969 (56%); Asia with 42 countries published the second most articles 13,163 (32%); and America with sixteen countries published the third most articles 12,333 (30%). Africa, and Oceania two continents made much less contributions, and the quantity of them were 933 (2.3%), and 667 (1.6%), respectively. It is noticeable that Europe is taking the leading position of thermodynamic research. Asia was seeing a striking increase to catch up with Europe in terms of scientific output (Friedberg, 2000; von Bubnoff, 2005).



**Figure 6.** Global geographical distribution of thermodynamics research outputs

### 3.3.2. Characteristics of top 20 countries/territories

With respect to international collaboration, 33,234 (81%) were independent publications and 7,748 (19%) were internationally collaborative publications. The collaboration rate was a little greater than that of other areas, such as 14% biosorption technology for water treatment (Ho, 2008), 16% of desalination research (Tanaka & Ho, 2011), 16% of solid waste research (Fu et al., 2010), and 14% of acupuncture research (Han & Ho, 2011). Table 4 shows the characteristics of the top 20 productive countries. The eight major industrialized countries G8, ranked in the top 11 in Table 4, had 59% over the investigation period. Similarly, the seven major industrialized countries G7 the USA, Germany, the UK, Japan, France, Canada, and Italy accounted for a significant proportion existed in many researches (Li et al., 2009; He, 2009; Fu et al., 2010; Wang et al., 2010). The USA dominated, ranking 1<sup>st</sup> in independent and collaborative articles, as well as first author and corresponding author articles. Total 1,421 contributing institutions (13%) were affiliated with USA, followed by China (824 institutions, 7.7%), and Russia (792 institutions, 6.5%). The 2<sup>nd</sup> position China, the 7<sup>th</sup> position India, and the 19<sup>th</sup> position Iran had low percentages of collaboration less than 20%. It was not coincident that China emerged as a leading nation in science production (Zhou & Leydesdorff, 2006; Zhou & Leydesdorff, 2008). In most fields, the USA had the quantity (number of papers) lead, although the China has made dramatic strides to overtake the USA, except the biomedical field and some aspects of environmental science (Kostoff, 2008).

Country	IN	TP	TP R (%)	SP R (%)	CP R (%)	FP R (%)	RP R (%)	%C
USA	1,421	9,162	1 (22)	1 (20)	1 (33)	1 (19)	1 (18)	28
China	824	4,652	2 (11)	2 (12)	5 (10)	2 (11)	2 (11)	17
Russia	792	3,792	3 (9.3)	3 (9.1)	6 (10)	3 (8.2)	3 (8.6)	20
Germany	724	3,421	4 (8.3)	6 (5.5)	2 (21)	4 (6.3)	4 (6.2)	47
Japan	580	2,804	5 (6.8)	4 (6.3)	7 (9.0)	5 (5.8)	5 (5.8)	25
France	792	2,515	6 (6.1)	7 (4.1)	3 (15)	7 (4.6)	7 (4.5)	46
India	652	2,201	7 (5.4)	5 (5.7)	15 (3.8)	6 (5.1)	6 (5.0)	13
Italy	390	1,858	8 (4.5)	8 (3.6)	8 (8.6)	8 (3.8)	8 (3.8)	36
UK	315	1,797	9 (4.4)	9 (2.5)	4 (12)	9 (3.0)	9 (2.9)	53
Spain	210	1,487	10 (3.6)	11 (2.5)	9 (8.4)	10 (2.9)	10 (2.8)	44
Canada	192	1,446	11 (3.5)	10 (2.5)	10 (7.8)	11 (2.7)	11 (2.6)	42
Poland	171	934	12 (2.3)	12 (1.6)	11 (5.1)	12 (1.7)	12 (1.7)	42
Netherlands	145	741	13 (1.8)	18 (1.1)	13 (4.7)	17 (1.3)	19 (1.2)	50
Brazil	196	733	14 (1.8)	14 (1.5)	19 (3.1)	13 (1.5)	13 (1.5)	33
Ukraine	229	720	15 (1.8)	15 (1.4)	18 (3.1)	14 (1.4)	14 (1.4)	34
Switzerland	111	690	16 (1.7)	21 (0.93)	12 (4.9)	19 (1.2)	18 (1.2)	55
Sweden	106	645	17 (1.6)	19 (1.1)	16 (3.5)	20 (1.2)	20 (1.1)	42
South Korea	176	632	18 (1.5)	17 (1.3)	22 (2.5)	16 (1.3)	16 (1.4)	31
Iran	173	587	19 (1.4)	13 (1.5)	32 (1.0)	15 (1.4)	15 (1.4)	14
Australia	106	566	20 (1.4)	23 (0.79)	14 (3.9)	21 (1.0)	21 (1.0)	54

IN: Number of institutions.

**Table 4.** Characteristics of the top 20 productive countries/territories

Besides, the 9<sup>th</sup> position UK, the 13<sup>th</sup> position Netherlands, the 16<sup>th</sup> position Switzerland, and the 20<sup>th</sup> position Australia had high cooperation rates no less than 50%. It was also reported that international collaboration in both within and outside the European Communities played an increasing role for European scientific literature (Narin et al., 1991; Glänzel, 1999). South Korea and Iran had higher rankings in terms of FP and RP than that of TP, while Netherlands and Sweden had lower rankings in terms of FP and RP. Moreover, from the above languages analysis, except English, the popular languages (Russian, Chinese, French, Japanese, and German) were just the mother tongue of the top five countries China, Russia, Germany, Japan, and France except the USA. The excellent performance of these countries was consistent with the results of language analysis.

### 3.3.3. Comparison of top six countries

The comparison of top six countries with the most articles in 2010 is illustrated in Fig. 7. The USA hold the trump card based on the total number of articles in the study period, but did not have the highest growth rate. China which was ranked 1<sup>st</sup> according to the 2010 production had the highest growth rate of 32 articles per year, and surpassed the USA in 2009, following distantly by other countries. USA, India, and Russia had the lower growth

rate of 10 - 13 articles per year. The following Germany and France had the growth rate of 6.3 and 5.9 articles per year. Particularly, Russia experienced a sharply increase in the first three year from 6 articles in 1991 to 174 articles in 1993, may due to its large fund for recovery of the politic reason (Goodman, 1993; Webb, 1994). The Russian annual output grew from 1980 to 1990, but fell after the dissolution of the USSR in late 1991; from 1994 there has been an inconsistent partial recovery, and by 2000 the annual output had approximately regained its 1980 value (Wilson & Markusova, 2004). It seems that the recovery time of Russian thermodynamic research was shorter.

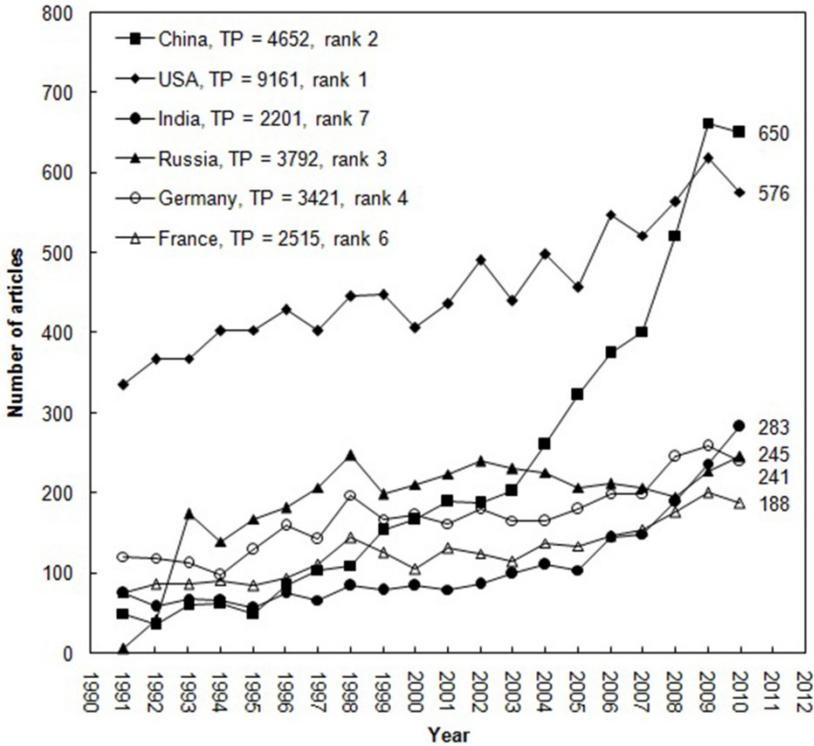
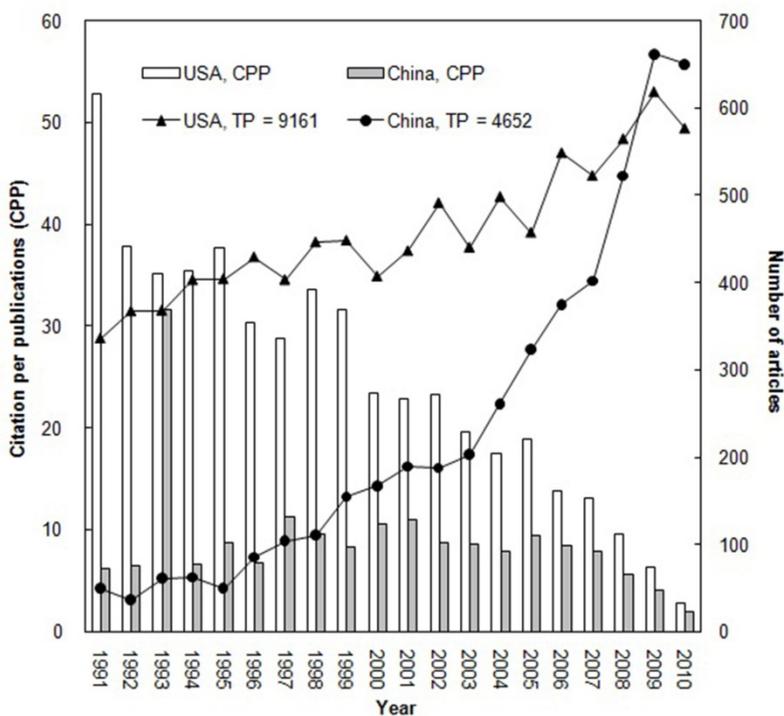


Figure 7. Trends of top six countries with most articles in 2010

### 3.3.4. Comparison of China and USA

In order to compare the most productive country in 1991-2010, the USA and the most active country in 2010, China, annual number of articles and citations per publication (CPP) of both were presented in Fig. 8. Total citations were collected on November 20 in 2011 from web of Science. From the above analysis, China experienced a high grow rate and got ahead of the USA in 2009 and kept on top in 2010. However, in terms of CPP, the mean number of China was 7.1 which was much less than that of the USA (23). The annual CPP of the USA showed a declined trend in 1991-2010, ranging from 53 in 1991 to 2.8 in 2010. Except the year

of 1993, the annual CPP of China fluctuated ranging 6.2-11 in 1991-2006, and decreased after 2007 down to 1.9 in 2010. Both countries indicated declines as for annual CPPs, which can be attributed to that it needs time to accumulate their citations (Picknett & Davis, 1999). The outstanding performance of China's CPP in 1993 might be owned to the two highly cited articles of a series by the same authors. They were "thermodynamics of molecular recognition by cyclodextrins. 1. calorimetric titration of inclusion complexation of naphthalenesulfonates with  $\alpha$ -,  $\beta$ -, and  $\gamma$ -cyclodextrin: enthalpy entropy compensation" (Inoue et al., 1993a) with 344 citations and "thermodynamics of molecular recognition by cyclodextrins. calorimetric titration of inclusion complexation with modified  $\beta$ -cyclodextrins. enthalpy-entropy compensation in host-guest complexation: from ionophore to cyclodextrin and cyclophane" (Inoue et al., 1993b) with 198 citations, respectively. Furthermore, the most frequently cited article was "a modified UNIFAC model. 2. present parameter matrix and results for different thermodynamic properties" (Gmehling et al., 1993) with 727 citations. Although this article was published by authors from Germany only, it was also assigned to China according to its address record from Web of Science, because one of the authors had permanent address of China. It is a bias of address information for articles from Web of Science. China's CPP in 1993 were still high (CPP = 20) without these highest citations articles. Likewise, the well performance of the USA's CPP in 1991 can be ascribed to the top cited article "protein folding and association: insights from the interfacial and thermodynamic



**Figure 8.** Comparison of USA and China by number of articles and citations per publication

properties of hydrocarbons” which was published in 1991 (Nicholls et al., 1991) and received 4,999 citations. Most scientific publications from China have a lower citation impact than the world average and have a lower citation rate than expected (Glänzel et al., 2002). It is suggested that China’s science needs to move from the “quantitative expansion” phase in nowadays to a “rising quality” phase (Jin & Rousseau, 2005). In general, China showed a high growth rate in recent years and dominant now in annual production, but still needs to make efforts on increasing their citations in thermodynamics.

### 3.4. Institutional contributors

#### 3.4.1. Characteristics of top 20 institutions

After examining the national contributors, the characteristics of institutional contributors institutions were identified. Of 40,982 articles from 10,696 institutions in 128 countries, 16,628 (41%) were inter-institutionally collaborative publications, and 24,354 (59%) were independent publications. The percentage of collaboration among institutions was much higher than that among countries (19%). The inter-institutional collaboration rate was usually greater than international collaboration rates (Fu et al., 2010; Han & Ho, 2011; Li et al., 2011; Tanaka & Ho, 2011). The number of articles of institutions was smaller than the country, and it was reported that the collaboration was more likely to happen when the size of actors was small (Narin et al., 1991). Nevertheless, the inter-institutional collaboration rate (41%) of thermodynamic research was observed to be lower than that of many other fields, such as 62% of global climate change (Li et al., 2011), 53% in atmospheric simulation (Li et al., 2009), 44% in solid waste research (Fu et al., 2010), and 53% of acupuncture research (Han & Ho, 2011). Four institutions in the USA and Japan, three in China, two each in Russia, and one each in Sweden, Ukraine, UK, India, France, and Italy were ranked in the top 20 productive institutions (16%) as shown in Table 5. It is worth noting that the Russian Academy of Sciences ranked 1<sup>st</sup> and Chinese Academy of Sciences ranked 2<sup>nd</sup> are both integrated research centers and made up of many relatively independent institutions distributed throughout their country. At present, the publications of these institutions were pooled as one heading, and publications divided into branches would result in different rankings. A bias appeared because national research institutions might have many branches in different cities, for example the CAS (Li et al., 2009), the RAS (Li et al., 2009), and Indian Institute of Technology (Tanaka & Ho, 2011). RAS founded the most productive thermodynamic journal of *Russian Journal of Physical Chemistry A*. In particular, 228 articles (28%) were contributed by RAS, and 117 articles (14%) were contributed by Moscow Lomonosov State University in Russia based on the total articles (817 articles with author information) of *Russian Journal of Physical Chemistry A* during 1991-2010. With the exception of these two institutions, the most productive institution is Moscow Lomonosov State University in Russia (425; 1.0%), followed by Tohoku University in Japan (335; 0.82%), and Centre National de la Recherche Scientifique in France (313; 0.76%). However, a bias would appear in the analysis of institutions which was used by different names in their publications. It is strongly recommended that an “international identity number” for all institutions when authors published their paper with an institution as affiliation in a Web of Science-listed journal (Chiu & Ho, 2007).

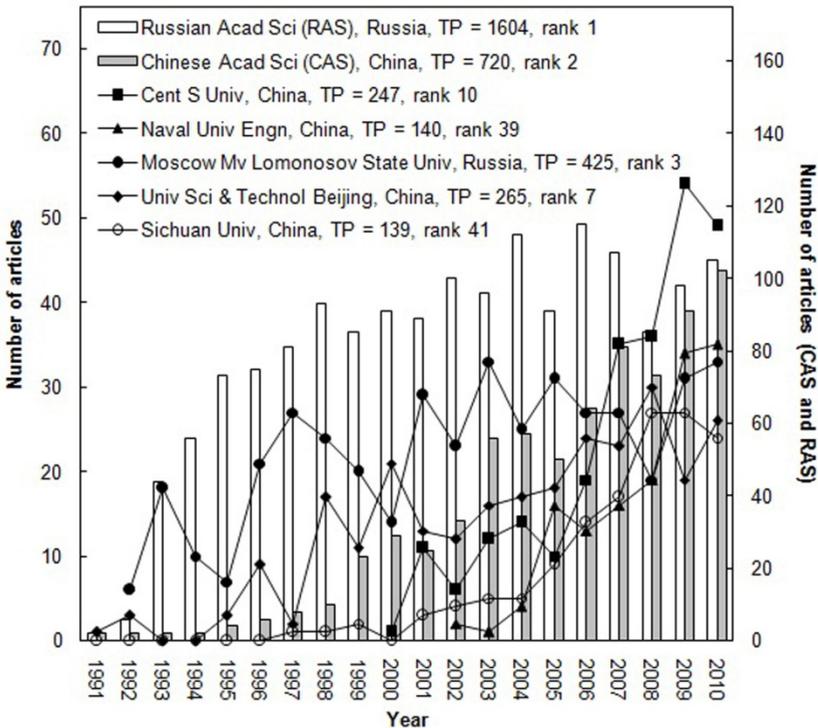
Institution	TP	TP R (%)	SP R (%)	CP R (%)	FP R (%)	RP R (%)	% C
Russian Academy of Sciences, Russia	1,604	1 (3.9)	1 (3.7)	1 (4.2)	1 (3.0)	1 (3.1)	43
Chinese Academy of Sciences, China	720	2 (1.8)	3 (0.92)	2 (3.0)	2 (1.1)	2 (1.1)	69
Moscow Lomonosov State University, Russia	425	3 (1.0)	2 (0.93)	5 (1.2)	3 (0.75)	3 (0.80)	47
Tohoku University, Japan	335	4 (0.82)	10 (0.52)	4 (1.3)	8 (0.46)	7 (0.45)	62
Centre National de la Recherche Scientifique, France	313	5 (0.76)	23 (0.34)	3 (1.4)	11 (0.41)	13 (0.39)	73
University of Tokyo, Japan	280	6 (0.68)	6 (0.57)	11 (0.84)	6 (0.46)	6 (0.45)	50
University of Science and Technology Beijing, China	265	7 (0.65)	9 (0.53)	14 (0.82)	5 (0.47)	5 (0.48)	52
Royal Institute of Technology, Sweden	261	8 (0.64)	14 (0.45)	7 (0.91)	12 (0.41)	11 (0.40)	58
Pennsylvania State University, USA	256	9 (0.62)	5 (0.58)	19 (0.69)	9 (0.45)	10 (0.43)	45
Central South University, China	247	10 (0.60)	11 (0.51)	18 (0.74)	4 (0.50)	4 (0.52)	50
University of Wisconsin-Madison, USA	245	11 (0.60)	14 (0.45)	15 (0.81)	14 (0.41)	18 (0.37)	55
Indian Institute of Technology, India	242	12 (0.59)	4 (0.67)	42 (0.48)	6 (0.46)	8 (0.44)	33
University of California, USA	241	13 (0.59)	18 (0.39)	8 (0.88)	16 (0.39)	22 (0.33)	61
Osaka University, Japan	240	14 (0.59)	16 (0.41)	11 (0.84)	17 (0.37)	15 (0.38)	58
Massachusetts Institute of Technology, USA	222	15 (0.54)	8 (0.55)	35 (0.53)	10 (0.42)	11 (0.40)	40
University of Cambridge, UK	220	16 (0.54)	29 (0.30)	8 (0.88)	22 (0.34)	24 (0.33)	66
Polish Academy of Sciences, Poland	219	17 (0.53)	24 (0.33)	13 (0.83)	22 (0.34)	21 (0.35)	63
National Research Council, Italy	208	18 (0.51)	166 (0.11)	6 (1.1)	52 (0.20)	58 (0.19)	87
National Academy of Sciences of Ukraine, Ukraine	201	19 (0.49)	7 (0.57)	80 (0.37)	12 (0.41)	9 (0.43)	31
Kyoto University, Japan	200	20 (0.49)	18 (0.39)	27 (0.63)	18 (0.36)	17 (0.37)	53

**Table 5.** Characteristics of the top 20 productive institutions.

More independent institutions might lead to more first author articles and corresponding author articles or vice versa. Some institutions which had low collaboration rates no more than 40% usually had a higher rank in FP and RP. For example, the 12<sup>th</sup> place Indian Institute of Technology in India with the low collaboration rate of 33% ranked 6<sup>th</sup> in FP and 8<sup>th</sup> in RP; the 15<sup>th</sup> position Massachusetts Institute of Technology in USA with the low collaboration rate of 40% ranked 10<sup>th</sup> in FP and 11<sup>th</sup> in RP; the 19<sup>th</sup> position National Academy of Sciences of Ukraine in Ukraine with the low collaboration rate of 31% ranked 12<sup>th</sup> in FP and 9<sup>th</sup> in RP. On the other hand, some institutions which had high collaboration rates more than 70% were ranked lower in the rankings of FP and RP. For example, the 5<sup>th</sup> position Centre National de la Recherche Scientifique in France with the high collaboration rate of 73% ranked 11<sup>th</sup> in FP and 13<sup>th</sup> in RP; the 18<sup>th</sup> position National Research Council in Italy with the high collaboration rate of 87% ranked 52<sup>th</sup> in FP and 58<sup>th</sup> in RP.

### 3.4.2. Comparison of top seven institutions

To identify the growth trends of active institutions in recent years, the trends of top seven productive institutions with most articles in 2010 are shown in Fig. 9. The most productive institution - RAS had an overwhelming majority in the total articles, and CAS was just down by three articles in 2010, following distantly by the other institutions. CAS as the China's highest academic institution in natural sciences played an active role in terms of scientific outputs in recent years as the exponentially growth scientific production in China (Li et al., 2009; Fu et al., 2010; Tanaka & Ho, 2011; Fu et al., 2011; Li et al., 2011).



**Figure 9.** Trends of top seven institutions with most articles in 2010

Although three universities in China including Central South University, Naval University of Engineering, and SiChuan University just ranked 10<sup>th</sup>, 39<sup>th</sup>, and 43<sup>rd</sup> of total articles from 1991 to 2010, but they had high rankings (3<sup>rd</sup>, 4<sup>th</sup>, and 7<sup>th</sup>) with respect to the number of articles in 2010. The growth rates of the top institutions differed from each other. Particularly, based on the last decade (2001-2010), CAS showed the highest growth rate of 7.2 articles per year; CSU and NUE showed the growth rate of 4 – 5 articles per year. The other four institutions, RAS, Moscow Lomonosov State University, University of Science and Technology Beijing, and SiChuan University showed the growth rate of 1 – 2 articles

per year. About 14% percent articles in RAS were published in *Russian Journal of Physical Chemistry A* which was founded by RAS. It was interesting that the top three institutions (CAS, CSU, and NUE) with the greatest growth rates were all in China. CSU was established in 2000 by merging three separate universities: Hunan Medical University, Changsha Railway University, and Central South University of technology, and was involved in “985 Project” and “211 Project” which were supported by Chinese government to promote the development and reputation of the Chinese higher education system (<http://iecd.csu.edu.cn/en-US/ColumnS.aspx?cid=12>). Moreover, CSU hold one SCI journal named *Transactions of Nonferrous Metals Society of China* which published 11% thermodynamic related articles of CSU in the study period. Another institution, NUE ranks as a military university of higher learning subjected to the leadership of the Central Military Commission and the Party Committee of the PLA Navy, and is listed as one of the five comprehensive universities in the armed forces and the army “2110 project” that enjoys the priority in development. It falls into the category of key national university specializing in engineering ([http://english.chinamil.com.cn/site2/special-reports/2007-06/21/content\\_853791.htm](http://english.chinamil.com.cn/site2/special-reports/2007-06/21/content_853791.htm)).

### 3.5. Research emphases and trends

Bibliometric analysis of author keywords has been only observed in recent years (Chiu & Ho, 2007; Wang et al., 2010; Li et al., 2011). It tried to find the research emphases and trends by quantitatively analyzing the frequency of author keywords. Excluding some articles without author keywords information, 23,458 articles (57%) with records of author keywords in the SCI-Expanded database were analyzed. There were 45,182 author keywords listed by authors, 43,930 (97%) keywords were used no more than ten times, which indicated that thermodynamic research involved diverse scientific literature and a wide disparity in research focuses (Chuang et al., 2007). Only 74 (0.16%) author keywords were used no less than 100 times, suggesting that the mainstream research in thermodynamics was considered to focus on a small field. Four five-year intervals (1991-1995, 1996-2000, 2001-2005, and 2006-2010) were employed to obtain the trends of these author keywords as well as minimize the year-to-year fluctuations. The top 30 author keywords (accounting for 37% of the total articles) in the latest interval 2006-2010 are listed in Table 6.

Except the author keywords “thermodynamics”, “thermodynamic properties”, “thermodynamic parameters”, and “thermodynamic” related to searching keywords, the three most frequently used author keywords were “kinetics” (883; 3.8%), “adsorption” (736; 3.1%), and “phase diagram” (545; 2.3%). “Thermodynamics” and “kinetics” were related to one another in ways, and were both commonly used to describe process (Kocks et al., 1975; Astumian, 1997; Ho & Ofomaja, 2005). “Adsorption” was a widely applied process, for example in environmental science (Wang et al., 2010; Wang et al., 2011; Chuang et al., 2011). The term “phase diagram” is a type of chart used to obtaining thermodynamic data at equilibrium (Kleppa, 1952; Svirbely, 1954).

Author keywords	TP	1991-2010 R (%)	1991-1995 R (%)	1996-2000 R (%)	2001-2005 R (%)	2006-2010 R (%)
thermodynamics	5,943	1 (25)	1 (31)	1 (25)	1 (23)	1 (25)
thermodynamic properties	1,577	2 (6.7)	2 (5.5)	2 (8.4)	2 (5.9)	2 (6.7)
kinetics	883	3 (3.8)	6 (2.5)	8 (2.2)	3 (3.6)	3 (4.8)
adsorption	736	5 (3.1)	11 (1.5)	10 (1.9)	6 (2.5)	4 (4.4)
thermodynamic parameters	778	4 (3.3)	3 (2.6)	3 (3.5)	4 (3.2)	5 (3.5)
thermodynamic phase diagram	503	9 (2.1)	26 (1.0)	15 (1.3)	10 (2.1)	6 (2.7)
entropy	545	7 (2.3)	21 (1.2)	6 (2.3)	9 (2.1)	7 (2.7)
thermodynamic modeling	548	6 (2.3)	8 (2.0)	7 (2.2)	7 (2.5)	8 (2.4)
thermodynamic analysis	338	13 (1.4)	165 (0.27)	56 (0.50)	16 (1.3)	9 (2.2)
heat capacity	385	11 (1.6)	12 (1.5)	14 (1.7)	12 (1.3)	10 (1.8)
calorimetry	533	8 (2.3)	3 (2.6)	5 (2.7)	5 (2.8)	11 (1.7)
phase diagrams	503	9 (2.1)	5 (2.5)	4 (3.0)	8 (2.2)	12 (1.7)
CALPHAD	260	17 (1.1)	26 (1.0)	31 (0.68)	25 (0.83)	13 (1.5)
solubility	186	25 (0.79)	N/A	782 (0.068)	35 (0.66)	14 (1.3)
enthalpy	325	14 (1.4)	10 (2.0)	16 (1.3)	13 (1.3)	14 (1.3)
thermodynamic property	373	12 (1.6)	8 (2.0)	9 (1.9)	11 (1.7)	16 (1.3)
density functional theory	212	20 (0.90)	59 (0.59)	64 (0.45)	25 (0.83)	17 (1.2)
isothermal titration calorimetry	158	36 (0.67)	1288 (0.045)	415 (0.11)	56 (0.53)	18 (1.1)
thermodynamic stability	177	28 (0.75)	1288 (0.045)	108 (0.34)	31 (0.70)	19 (1.1)
isotherm	265	16 (1.1)	38 (0.77)	16 (1.3)	13 (1.3)	20 (1.0)
equation of state	120	60 (0.51)	1288 (0.045)	565 (0.09)	231 (0.18)	21 (1.0)
density	316	15 (1.3)	7 (2.4)	13 (1.7)	13 (1.3)	21 (1.0)
molecular dynamics	178	27 (0.76)	29 (1.0)	41 (0.59)	60 (0.51)	23 (0.94)
free energy	172	29 (0.73)	165 (0.27)	31 (0.68)	47 (0.61)	24 (0.93)
phase equilibria	163	33 (0.69)	165 (0.27)	52 (0.52)	51 (0.59)	25 (0.92)
biosorption	228	19 (1.0)	32 (0.86)	25 (0.83)	18 (1.2)	26 (0.91)
AB initio calculations	101	72 (0.43)	N/A	N/A	431 (0.11)	27 (0.89)
phase transition	121	59 (0.52)	N/A	170 (0.25)	147 (0.26)	27 (0.89)
nonequilibrium thermodynamics	158	36 (0.67)	52 (0.64)	58 (0.47)	60 (0.51)	29 (0.86)
	190	24 (0.81)	23 (1.1)	27 (0.81)	39 (0.64)	30 (0.85)

N/A: Not Available

**Table 6.** The most frequently used 30 author keywords in 2006-2010

In particular, there were also some emerging hotspots in thermodynamics recently. Some author keywords including the 3<sup>rd</sup> “adsorption”, the 9<sup>th</sup> “thermodynamic modeling”, the 14<sup>th</sup> “CALPHAD”, the 17<sup>th</sup> “thermodynamic property”, the 18<sup>th</sup> “density functional theory”, the 19<sup>th</sup> “isothermal titration calorimetry”, the 20<sup>th</sup> “thermodynamic stability”, the 21<sup>st</sup> “isotherm”, the 25<sup>th</sup> “free energy”, the 27<sup>th</sup> “biosorption”, and the 28<sup>th</sup> “AB initio calculations” in the list showed the increasing trends during the study period. It is noticeable that “CALPHAD”, “biosorption”, and “AB initio calculations” increased rapidly from zero articles in 1991-1995 into the top 30 rankings in 2006-2010. “CALPHAD” was firstly used as the author keyword of the article entitled “compilation of ‘CALPHAD’ formation enthalpy data - Binary intermetallic compounds in the COST507 Gibbsian database” in 1998 (Fries & Jantzen, 1998). However, “CALPHAD method” had been used as the author keyword of the article titled “thermodynamic study on the Ag-Sb-Sn system” in 1996 (Oh et al., 1996). The first article which employed “biosorption” as author keyword was titled “determination of the equilibrium, kinetic and thermodynamic parameters of the batch biosorption of nickel(II) ions onto *Chlorella vulgaris*” in *Process Biochemistry* in 2002 (Aksu, 2002). “Biosorption” as a process for water treatment received increasing attention in recent years (Ho, 2008). As for “AB initio calculations”, it was originally utilized as author keywords of the article “an AB initio study of structures and energetics of copper sulfide clusters” in 1996 (Dehnen et al., 1996). Similarly, “density functional theory”, “isothermal titration calorimetry”, and “isotherm” grew fast from the 1288<sup>th</sup> (only one article) in 1991-1995 to 18<sup>th</sup>, 19<sup>th</sup>, and 21<sup>st</sup> in 2006-2010. The article targeting at “density functional theory” could be found in 1994 and it was entitled “density-functional theory as thermodynamics” (Nagy & Parr, 1994). Thermodynamical interpretation of the density functional theory for an electronic ground state was developed (Nagy & Parr, 1994). The following article which utilized “density functional theory” as author keyword was published in 1999. For the phrase “isothermal titration calorimetry”, the article which used it as author keyword appeared in 1995, and it was titled “comparative thermodynamic analyses of the Fv, Fab\* and Fab fragments of anti-dansyl mouse monoclonal-antibody” (Shimba, 1995). However, it should be noticed that there was a bias that all these analysis were based on the data (57%) with author keywords information from SCI-Expanded.

#### 4. Conclusion

Except the dominant language English, Russian, Chinese, French, Japanese and German were the most common languages. Above all, the growth process of annual thermodynamic scientific outputs can be divided into two stages, and the annual growth rate of the second stage 2004-2010 was four times of that in the first stage 1991-2003. Secondly, *Russian Journal of Physical Chemistry* was the most productive journal, and then *Journal of Alloys and Compounds* and *Journal of Chemical Physics*. The most common category was found to be physical chemistry. Thirdly, the global geographic distribution discovered that Europe took the leading position, following by Asia, America, Africa and Oceania. In particular, the eight major industrialized countries (G8: Canada, France, Germany, Italy, Japan, Russia, the UK, and USA) played a prominent role with more than a half contribution, especially the USA.

However, China experienced the greatest growth rate, and surpassed the USA in 2009 in terms of annual production, but needs to enhance its quality of publications. China and India had low collaboration rates while the UK, Netherlands, and Switzerland in Europe with a smaller size had high collaboration rates. In general, the thermodynamic research presented a higher international collaboration rate but a lower inter-institutional collaboration rate in comparison with other fields. Russian Academy of Sciences and Chinese Academy of Sciences took the leading position of institutions, following distantly by Tohoku University in Japan, and Centre National de la Recherche Scientifique in France. It was also revealed that the institutions with lower collaboration rates usually published greater proportion of first author articles and corresponding author articles, and vice versa. Finally, by analyzing the latest most frequently used author keywords, it was concluded that the items “thermodynamic properties”, “kinetics”, “adsorption”, “thermodynamic parameters”, “phase diagram”, and “entropy” are the traditional research hotspots and will continue being the emphases in the foreseeable future. “CALPHAD”, “density functional theory”, “isothermal titration calorimetry”, “isotherm”, “biosorption”, and “AB initio calculations”, as the quickly increasing concernings, are the newly thermodynamic research hotspots.

## Author details

Hui-Zhen Fu<sup>1</sup>, Yuh-Shan Ho<sup>1,2,\*</sup>

<sup>1</sup>Department of Environmental Sciences, Peking University, People's Republic of China

<sup>2</sup>Trend Research Centre, Asia University, Taiwan

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\* Corresponding Author

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