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Letter

Proposal of a Standard Unit for Turnover Frequencies: Hz

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Os autores deste manuscrito propõem que frequências de rotação sejam expressas em uma unidade do Sistema Internacional de Unidades já existente (Hz), facilitando a comparação entre diferentes sistemas catalíticos.

The authors of this manuscript propose turnover frequencies to be expressed in an International System of Units existing unit (Hz), facilitating the comparison between different catalytic systems.

Keywords: heterogeneous catalysis, homogeneous catalysis, kinetics, turnover frequency, units

Since the Greek civilization, humanity has been dealing with measurement as a science. Originally, measures were taken as multiples of a known object like a foot or an inch. After the French revolution, the French government imposed the metric system as an attempt to standardize measurements, although its use is not yet spread all over the world, especially in countries originated from the former British Empire. Nevertheless, throughout the 20th century, the metric system has established itself as the International System of Units incorporated it and some other basic units to allow the measurement of virtually all magnitudes on nature.[1] Derived units such as joule, watt and hertz (Hz) are used to make simpler the expression of quantities, facilitating their use and comparison.

In catalysis, even in present days, we also face a lack of uniformity when expressing a very useful parameter for the efficiency of a catalytic system: turnover frequencies (TOFs). This parameter is also sometimes called "activity", especially in polymerization and is used to refer to the number of moles of substrate that can be converted *per* mole of catalyst *per* unit of time. In the literature, we usually find this presented with the dimension time^{-1}, but

Table 1. Data collected from the 15 most recent papers on ISI database (May 5th, 2014) having "turnover frequency" as a topic

Reaction	Catalyst	Max. TOF	Unit	Ref.
Nitroarenes hydrogenation	[Pt/Fe]	500	h^{-1}	3
Cyclohexene oxidation	[V]	14465	h^{-1}	4
Polilactic acid depolimerization	Biogenic creatinine	347.7	h^{-1}	5
Aromatic compounds hydrogenation	Ir nanoparticles	3215	h^{-1}	6
Ethanol/acetaldehyde reforming	$Cu/Ni/SiO_2$	0.0063	s^{-1}	7
CO_2 methanation	Ni/SiO_2-nanoparticles	1.61	s^{-1}	8
Ammonia borane dehydrogenation	Pd/SiO_2-$CoFe_2O_4$	254	min^{-1}	9
Water oxidation	Au/MnO_x	0.01	s^{-1}	10
Alkenes epoxidation	[Ru]	24120	h^{-1}	11
Ethane oxidation	[Co]	3.35×10^{-21}[a]	s^{-1}	12
Ammonium salts carbonilation	[Pd]	1289	h^{-1}	13
Water reduction	[Co]	3200	h^{-1}	14
Water oxidation	Hydrous iron oxide	2900	s^{-1}	15
Fisher-Tropsch	Co nanoparticles	0.2	s^{-1}	16
Water-gas shift	Pt/CeO_2	0.2	s^{-1}	17

[a]Theoretical value.

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Table 2. Data collected from the 15 most cited papers (May 5th, 2014) on ISI database which have "turnover frequency" as a topic. TOF presented is the highest reported

Reaction	Catalyst	Max. TOF	Unit	Ref.
Primary alcohols oxidation	$Au-Pd/TiO_2$	270000	h^{-1}	18
Insaturated amines hydroamination	Organolanthanides	7600	h^{-1}	19
CO oxidation	[Au]/supports	6.7	s^{-1}	20
CO oxidation	Co_3O_4 nanorods	7.45×10^{-2}	s^{-1}	21
Styrene hydroformylation	[Rh]	4285	h^{-1}	22
Aminolefins hydroamination	Organolanthanides	200	h^{-1}	23
Sonogashira coupling	[Pd]	205	h^{-1}	24
Ethylene polymerization	[Ni]	2800×10^{-3}	h^{-1}	25
Alcohols oxidation	[Pd]/hidroxyapatite	9800	h^{-1}	26
Fischer-Tropsch	Co/C	34.8×10^{-3}	s^{-1}	27
Bromoarenes and boranes coupling	Pd/graphene oxide	39000	h^{-1}	28
Ethylene polymerization	[Zr]	42900	s^{-1}	29
Supercritical CO_2 hydrogenation	[Ru]	1500	h^{-1}	30
Aryl halides Heck vinylation	Paladacycles	20000	h^{-1}	31
Methane oxidation	Hg	10^{-3}	s^{-1}	32

the unit of time is not standardized. A search performed on ISI database[2] tagging "turnover frequencies" and retaining the 15 most recent papers listed serves as a sample of this non-uniformity, as shown in Table 1.

In order to show that this is not only a recent discrepancy, we also performed a research considering the 15 most cited papers on ISI database using the same tag, on the same day (Table 2).

It becomes then unnatural for a researcher to compare different catalytic systems without calculations. By using Hz, an existing unit which expresses cycles *per* second, this comparison becomes immediate, as shown in Table 3, where reactions were grouped and TOFs recalculated having Hz as unit.

The use of Hz to express TOFs is not only a more elegant alternative, but it allows an immediate comparison of different catalytic systems under different conditions. It is also possible to use multiplicative prefixes. For example, for many relevant industrial applications, the turnover frequency varies between 10^{-2}-10^{2} s^{-1}, while it is in the range of 10^{3}-10^{7} s^{-1} for enzymes,[33] and these two data could be classified into mHz, Hz, kHz or MHz, highlighting distinct activities.

Thus, we propose the use of the standard unit of frequency hertz whenever TOFs and activities are referred, in order to facilitate comparison of scientific work and didactically consolidate even further the image of the catalytic cycle and the International System of Units.

Acknowlegments

This work is issued from an original idea of Prof Roberto F. de Souza. We had then selected data to translate his purpose

Table 3. Compared turnover frequencies expressed in Hz

Reaction type	Catalyst	Max. TOF / Hz	Ref.
Carbonylation	[Pd]	8.03×10^{-2}	13
Cross-coupling	[Pd]	5.69×10^{-2}	24
	Pd-graphene oxide	1.08×10	28
Dehydrogenation	$Pd/SiO_2-CoFe_2O_4$	4.23	9
Depolymerization	Biogenic creatinine	9.66×10^{-2}	5
Epoxidation	[Ru]	6.70	11
Fischer-Tropsch	Co nanoparticles	2.00×10^{-1}	16
	Co/C	3.48×10^{-3}	27
Heck vinylation	Paladacycles	5.56	31
Hydroamination	Organolanthanides	2.11	19
	Organolanthanides	5.50×10^{-2}	23
Hydroformylation	[Rh]	1.19	22
Hydrogenation	[Pt/Fe]	1.39×10^{-1}	3
	Ir nanoparticles	8.93×10^{-1}	6
	[Ru]	4.17×10^{-2}	30
Methanation	Ni/SiO_2-nanoparticles	1.61	8
Oxidation	[V]	4.02	4
	Au/MnO_x	1.00×10^{-2}	10
	[Co]	3.35×10^{-21}	12
	Hydrous Fe oxide	2.90×10^{3}	15
	$Au-Pd/TiO_2$	7.5×10	18
	[Au] supported	6.70	20
	Co_3O_4 nanorods	7.45×10^{-2}	21
	[Pd]/hydroxyapatite	2.72	26
	Hg	1.00×10^{-3}	32
Polymerization	[Ni]	7.80×10^{-4}	25
	[Zr]	4.29×10^{4}	29
Reduction	[Co]	8.89×10^{-1}	14
Reforming	$Cu/Ni/SiO_2$	6.30×10^{-3}	7
Water-gas shift	Pt/CeO_2	2.00×10^{-1}	17

into a manuscript, but he left us in November 2013, leaving an enormous sensation of emptiness. Without him, we selected new data and to him we dedicate the development of his proposal. We hope to have honored his memory.

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