Advances in Dynamically Controled Catalytic Reaction Engineering

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Electronic Supplementary Information

Table S1 summarizes a comprehensive literature review of natural and forced catalytic oscillations. When reported, turnover frequencies (TOFs) at reaction temperatures are directly tabulated. In instances where no TOF was reported, a secondary source was identified at comparable conditions and denoted by superscripts in the respective columns. The effective Damkholer number $(Da_{eff} = TOF/f)$ was then calculated as the ratio TOF to forced oscillation frequency. The full data set is visualized in Figure 7 of the manuscript.

Table S1: Tabulated natural and forced oscillations observed in catalytic systems.

#	Reference	Reaction	Condition	Oscillation Type	Low Frequency (Hz)	High Frequency (hz)	Reaction specific TOF (hz)	Low Da (TOF/ Frequency)	High Da (TOF/ Frequency)
1	Brandner et al, 2004 ¹	CO Oxidation	Temperature	Forced	-	0.0166	0.033 ²	-	2
2	Luther et al, 2008 ³	CO Oxidation	Temperature	Forced	-	0.1	0.033 ²	-	0.333
3	Stolte et al, 2013⁴	CO Oxidation	Temperature	Forced	-	20	25	-	0.1
4	Jensen et al, 2007 ⁶	CO Oxidation	Temperature	Forced	0.02	1	0.033 ²	1.67	0.0333
5	Xu et al, 2018 ⁷	Rhodamine B Decomposition	Vibration	Forced	-	40000	2.5	-	0.0000625
6	Yukawa et al, 2002 ⁸	Ethanol Decomposition	Vibration	Forced	3500000	17400000	0.000033 ⁹	9.5E-12	1.92E-12
7	Muraki et al, 1985 ¹⁰	CO Oxidation	Concentration	Forced	0.05	10	0.053311	1.067	0.00533
8	Zhou et al, 1986 ¹²	CO Oxidation	Concentration	Forced	-	2	0.013311	-	0.00667
9	Graham and Lynch, 1990 ¹³	CO Oxidation	Concentration	Forced	0.0005	0.017	0.25	500	14.71
10	Zhou and Gulari, 1986 ¹⁴	CO Oxidation	Concentration	Forced	0.02	0.1	0.115	5	1
11	Hu et al, 1998 ¹⁶	Methane Oxidation	Reaction Induced	Natural	0.0001	0.01	0.0066717	66.67	0.667
12	Slavinskaya et al, 2011 ¹⁸	CO Oxidation	Reaction Induced	Natural	0.00416	0.033	0.053311	12.8	1.6
13	Hendriksen et al, 2010 ¹⁹	CO Oxidation	Reaction Induced	Natural	-	0.00066	0.0006675	-	75000
14	Kaichev et al, 2016 ²⁰	Propane Oxidation	Reaction Induced	Natural	-	0.00104	5.4	-	5184
15	Delikonstantis et al, 2020 ²¹	Non-Oxidative Methane Coupling	Plasma	Forced	3000	100000	0.0000122	3.3E-9	1.0E-10
16	Yao et al, 2001 ²³	Methane to Acetylene	Plasma	Forced	1000	8000	0.04524	4.5E-5	5.63E-6
17	Kado et al, 2003 ²⁵	Methane to Acetylene	Plasma	Forced	45	225	0.04524	0.0001	0.0002
18	Deng et al, 2014 ²⁶	Hydrogen Evolution Reaction	Voltage	Forced	20	70	3.93 ²⁷	0.196	0.0561
19	Ohkawara et al, 1996 ²⁸	Ethanol Oxidation	Voltage	Forced	-	84000	0.0031729	-	3.77E-8
20	Fu et al, 1984 ³⁰	Alkene Isomerization	Light	Forced	5	25	10000	2000	400
21	Pschenitza et al. 2016 ³¹	CO2 Reduction	Light	Forced	500	10000	0.003055	6.1E-6	3.06E-7

22	Yamani, 2018 ³²	Methylene Blue Decomposition	Light	Forced	-	10	1.1133	-	0.111
23	Kolbitsch et al, 2010 ³⁴	Combustion	Chemical Looping	Forced	0.0056	0.0415	11.9	2117.01	286.79
24	Naqvi et al, 2005 ³⁵	Combustion	Chemical Looping	Forced	-	0.00493	11.9	-	2415.7
25	Ryden et al, 2011 ³⁶	Combustion	Chemical Looping	Forced	0.00625	0.0175	11.9	1904	680
26	De Diego et al, 2008 ³⁷	Methane Combustion	Chemical Looping	Forced	0.000185	0.00204	11.9	64260	5841.8
27	Escudero et al, 2007 ³⁸	Oxygen Reduction	Impedance Spectroscopy	Forced	0.01	1000000	100	10000	0.0001
28	Wang and Rick, 2014 ³⁹	Lithium Ion Battery	Impedance Spectroscopy	Forced	0.01	1000	0.5	50	0.0005
29	Liang et al, 2015 ⁴⁰	$LiNi_{0.5}CO_{0.2}$ - $Mn_{0.3}O_2$ Capacitance	Impedance Spectroscopy	Forced	0.01	100000	20	2000	0.0002
30	Yoon et al, 2002 ⁴¹	PCR	PCR	Forced	0.00833	0.166	1.25	150	7.5
31	Woolley et al, 1996 ⁴²	PCR	PCR	Forced	-	0.033	1.25	-	37.5
32	Farrar and Wittwer, 2015 ⁴³	PCR	PCR	Forced	0.0485	1.25	1.25	25.75	1
33	Abulesz and Lyberatos, 198844	Yeast biomass production	Bioreactor	Forced	0.0000694	0.000138	0.0000842	1.21	0.606
34	Pickett and Bazin, 1979 ⁴⁵	E. Coli growth and composition	Bioreactor	Forced	0.0000463	0.00111	0.0000463	1	0.0417
35	Panic et al, 2011 ⁴⁶	Ferrocyanide electrooxidation	Frequency Response	Forced	0.01	10000	10	1000	0.001
36	Petkovska and Do, 199847	Langmuir kinetic simulation	Frequency Response	Forced	0.0000138	13.8	0.0138	1000	0.001

Supplemental Citations

- 1 J. J. Brandner, G. Emig, M. A. Liauw and K. Schubert, *Chem. Eng. J.*, 2004, **101**, 217–224.
- 2 M. Haneda, T. Watanabe, N. Kamiuchi and M. Ozawa, *Appl. Catal. B Environ.*, 2013, **142–143**, 8–14.
- 3 M. Luther, J. J. Brandner, L. Kiwi-Minsker, A. Renken and K. Schubert, *Chem. Eng. Sci.*, 2008, **63**, 4955–4961.
- J. Stolte, L. Özkan, P. C. Thüne, J. W. Niemantsverdriet and A. C. P. M. Backx, *Appl. Therm. Eng.*, , DOI:10.1016/j.applthermaleng.2012.06.035.
- 5 P. J. Berlowitz, C. H. F. Peden and D. W. Goodman, *Kinetics of CO Oxidation on Single-Crystal Pd, Pt, and I r,* 1988, vol. 92.
- 6 S. Jensen, J. L. Olsen, S. Thorsteinsson, O. Hansen and U. J. Quaade, *Catal. Commun.*, 2007, **8**, 1985–1990.
- 7 X. Xu, Y. Jia, L. Xiao and Z. Wu, 2018, **193**, 1143–1148.
- 8 Y. Yukawa, N. Saito, H. Nishiyama and Y. Inoue, in *Surface Science*, 2002, vol. 502–503, pp. 527–531.
- 9 P. Ferrin, D. Simonetti, S. Kandoi, E. Kunkes, J. A. Dumesic, J. K. Nørskov and M. Mavrikakis, , DOI:10.1021/ja8099322.

- 10 H. Muraki, H. Sobukawa and Y. Fujitani, *Nippon KAGAKU KAISHI*, 1985, **1985**, 176–181.
- 11 M. Haneda, M. Todo, Y. Nakamura and M. Hattori, *Catal. Today*, 2017, **281**, 447–453.
- 12 X. Zhou, Y. Barshad and E. Gulari, CO OXIDATION ON Pd/Al,O,. TRANSIENT RESPONSE AND RATE ENHANCEMENT THROUGH FORCED CONCENTRATION CYCLING, 1986, vol. 41.
- 13 W. R. C. Graham and D. T. Lynch, *AIChE J.*, 1990, **36**, 1796–1806.
- 14 X. Zhou and E. Gulari, *Chem. Eng. Sci.*, 1986, **41**, 883–890.
- 15 K. Murata, E. Eleeda, J. Ohyama, Y. Yamamoto, S. Arai and A. Satsuma, *Phys. Chem. Chem. Phys*, 2019, **21**, 18128.
- 16 Y. H. Hu and E. Ruckenstein*, , DOI:10.1021/IE980027F.
- 17 X. Zhang, S. D. House, Y. Tang, L. Nguyen, Y. Li, A. A. Opalade, J. C. Yang, Z. Sun and F. Feng Tao, , DOI:10.1021/acssuschemeng.8b00234.
- 18 E. M. Slavinskaya, O. A. Stonkus, R. V. Gulyaev, A. S. Ivanova, V. I. Zaikovskii, P. A. Kuznetsov and A. I. Boronin, *Appl. Catal. A Gen.*, 2011, **401**, 83–97.
- 19 B. L. M Hendriksen, M. D. Ackermann, R. van Rijn, D. Stoltz, I. Popa, O. Balmes, A. Resta, D. Wermeille, R. Felici, S. Ferrer and J. W. M Frenken, 2010, 11.
- V. V. Kaichev, D. Teschner, A. A. Saraev, S. S. Kosolobov, A. Y. Gladky, I. P. Prosvirin, N. A. Rudina,
 A. B. Ayupov, R. Blume, M. Hävecker, A. Knop-Gericke, R. Schlögl, A. V. Latyshev and V. I.
 Bukhtiyarov, J. Catal., 2016, 334, 23–33.
- 21 E. Delikonstantis, M. Scapinello, O. Van Geenhoven and G. D. Stefanidis, *Chem. Eng. J.*, 2020, **380**, 122477.
- 22 Y. Engelmann, P. Mehta, E. C. Neyts, W. F. Schneider and A. Bogaerts, ACS Sustain. Chem. Eng., 2020, 8, 6043–6054.
- 23 S. Yao, A. Nakayama and E. Suzuki, *AIChE J.*, 2001, **47**, 413–418.
- 24 Y. Xiao and A. Varma, ACS Catal., 2018, 8, 2735–2740.
- 25 S. Kado, K. Urasaki, Y. Sekine and K. Fujimoto, 2003, 1377–1385.
- 26 Q. Deng, M. Smetanin and J. Weissmüller, J. Catal., 2014, **309**, 351–361.
- 27 K. Jiang, B. Liu, M. Luo, S. Ning, M. Peng, Y. Zhao, Y.-R. Lu, T.-S. Chan, F. M. F. De Groot and Y. Tan, *Nat. Commun.*, 2019, **10**, 1743.
- 28 Y. Ohkawara, N. Saito and Y. Inoue, *Surf. Sci.*, 1996, **357–358**, 777–780.
- 29 F. Kaedi, Z. Yavari, M. Noroozifar and H. Saravani, J. Electroanal. Chem., 2018, 827, 204–212.
- 30 K.-Ji. Fu, R. L. Whetten and E. R. Grant, *Pulsed-Laser-Initiated Photocatalysis in the Liquid Phase*, 1984, vol. 23.
- 31 M. Pschenitza, S. Meister, A. von Weber, A. Kartouzian, U. Heiz and B. Rieger, *ChemCatChem*, 2016, **8**, 2688–2695.
- 32 Z. H. Yamani, B. Zain and H. Yamani, *Arab J Sci Eng*, 2018, **43**, 423–432.

- 33 X.-M. Song, J.-M. Wu and M. Yan, *Thin Solid Films*, 2009, **517**, 4341–4347.
- P. Kolbitsch, J. Bolhàr-Nordenkampf, T. Pröll and H. Hofbauer, Int. J. Greenh. Gas Control, 2010, 4, 180–185.
- 35 R. Naqvi, J. Wolf and O. Bolland, *Energy*, 2007, **32**, 360–370.
- 36 M. Rydén, A. Lyngfelt and T. Mattisson, Int. J. Greenh. Gas Control, 2011, 5, 356–366.
- L. F. de Diego, M. Ortiz, J. Adánez, F. García-Labiano, A. Abad and P. Gayán, *Chem. Eng. J.*, 2008, 144, 289–298.
- 38 M. J. Escudero, A. Aguadero, J. A. Alonso and L. Daza, J. Electroanal. Chem., 2007, 611, 107–116.
- 39 F. M. Wang and J. Rick, *Solid State Ionics*, 2014, **268**, 31–34.
- 40 C. Liang, L. Liu, Z. Jia, C. Dai and Y. Xiong, *Electrochim. Acta*, 2015, **186**, 413–419.
- 41 D. S. Yoon, Y.-S. Lee, Y. Lee, H. J. Cho, S. W. Sung, K. W. Oh, J. Cha and G. Lim, *Precise temperature* control and rapid thermal cycling in a micromachined DNA polymerase chain reaction chip, 2002, vol. 12.
- 42 A. T. Woolley, D. Hadley, P. Landre, A. J. deMello, R. A. Mathies and M. Allen Northrup, Functional Integration of PCR Amplification and Capillary Electrophoresis in a Microfabricated DNA Analysis Device, 1996, vol. 68.
- 43 J. S. Farrar and C. T. Wittwer, *Clin. Chem.*, 2015, **61**, 145–153.
- 44 E.-M. Abulesz and G. Lyberatos, *Biotechnol. Bioeng.*, 1988, **34**, 741–749.
- 45 A. M. Pickett and M. J. Bazin, 1979.
- 46 V. V Panic, T. R. Vidakovi C-Koch, M. Andri, M. Petkovska and K. Sundmacher, *J. Phys. Chem. C*, 2011, **115**, 17352–17358.
- 47 M. Petkovska and D. D. Do, *Nonlinear frequency response of adsorption systems: isothermal batch and continuous flow adsorbers*, 1998, vol. 53.