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Oxygen Partial Pressure and Oxygen Concentration Flammability: Can They Be Correlated?

ABSTRACT: NASA possesses a large quantity of flammability data performed in ISS airlock (30% Oxygen 526mmHg) and ISS cabin (24.1% Oxygen 760 mmHg) conditions. As new programs develop, other oxygen and pressure conditions emerge. In an effort to apply existing data, the question arises: Do equivalent oxygen partial pressures perform similarly with respect to flammability? This paper evaluates how material flammability performance is impacted from both the Maximum Oxygen Concentration (MOC) and Maximum Total Pressures (MTP) perspectives. From these studies, oxygen partial pressures can be compared for both the MOC and MTP methods to determine the role of partial pressure in material flammability. This evaluation also assesses the influence of other variables on flammability performance. The findings presented in this paper suggest flammability is more dependent on oxygen concentration than equivalent partial pressure.

KEYWORDS: partial pressure, gaseous oxygen, Maximum Oxygen Concentration (MOC), normoxic, flammability, elevated oxygen, enriched oxygen, NASA STD 6001 Test 1, propagation rate

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Background

To safely and successfully operate in enriched oxygen conditions, understanding material flammability is critical for NASA, commercial space flight companies, and industry alike. Previous space programs have acquired significant data in the Space Transportation System (STS) environment of 30% O₂ at 70.3 kPa (10.2 psia). This same environment is also currently being evaluated for the Crew Exploration Vehicle (CEV). A significant amount of additional flammability data exists at the International Space Station (ISS) worst-case cabin conditions of 24.1% O₂ at 191.4 kPa (14.7 psia). In a desire to leverage existing data, the question arises: Do materials perform similarly with respect to flammability as long as the partial pressure of oxygen remains equivalent? This question is not only relevant to NASA and space programs. In the oxygen related industry, the ability to apply existing flammability data to various manufacturing and operating conditions would be beneficial. It is important that the question be thoroughly answered, as the ability to apply existing data to alternate conditions could save significant resources both financially and with respect to time and schedule. The purpose of this paper is to compile relevant data to examine the dependence of flammability on partial pressure of oxygen and oxygen concentration.

Normoxic Conditions and Partial Pressure

Normoxic conditions maintain an equivalent partial pressure of oxygen in the atmosphere as would be found in that of air at sea level. This level of oxygen is important for human function, and therefore space vehicles are designed to provide normoxic or close to normoxic conditions.

The concept of partial pressure depends on the ideal gas law (Eq. (1)):

$$PV = nRT \quad (1)$$

Where P = pressure; V = volume; n = moles of a molecule; R = ideal gas constant; and T = Temperature.

Assuming the ideal gas law, the partial pressure of oxygen p_{O_2} is defined as the pressure that would be exerted by n_{O_2} moles of O₂ alone in the same total volume V at the same temperature T (Eq. (2)).

$$p_{O_2} V = n_{O_2} RT \quad (2)$$

Dividing the second equation by the first yields that the mole fraction of a given component in a mixture times the total pressure will give you the component's partial pressure (Eq. (3) and Eq. (4)).

$$n_{O_2}/n = p_{O_2}/P \quad (3)$$

$$(n_{O_2}/n) * P = p_{O_2} \quad (4)$$

A similar calculation can be done for the pure component volume of a mixture. In an ideal gas mixture, a component's percentage by volume is equal to its mole fraction (Eq. (5) and Eq. (6)).

$$n_{O_2}/n = v_{O_2}/V \quad (5)$$

$$(n_{O_2}/n)*V = v_{O_2} \quad (6)$$

Therefore, referring to a gas mixture by its volume percent (e.g., 21% volume O₂) is the same as referring to it by its mole percent (21 mole % O₂). Assuming an ideal gas behavior, partial pressure can easily be calculated from volume fraction (Eq. (7) and Eq. (8)) [1].

$$p_{O_2} = (v_{O_2}/V)*P \quad (7)$$

$$\text{and conversely } (v_{O_2}/V) = p_{O_2}/P \quad (8)$$

Using this calculation, Table 1 outlines examples of normoxic environmental conditions that maintain equivalent partial pressures across a range of conditions.

The STS and the currently in-design CEV have resided at the 30% O₂ at 70.3 kPa (10.2 psia) point of the normoxic curve. The ISS aims to operate at the 21% O₂, 101.4 kPa (14.7 psia) point of the curve.

Nonetheless, it has obtained much of its data at 24.1% O₂, 101.4 kPa (14.7 psia) conditions due to sinusoidal fluctuations of oxygen with a mean of 21% O₂ seen on the ISS. Future long duration habitation modules might select to operate at lower pressure normoxic conditions to minimize time loss and health risk associated with frequent depressurizations when frequently exiting habitats. In addition, low pressure environments also provide structural design benefits for long-duration habitats. Use of Extravehicular Activity (EVA) suits is another scenario in which a reduced pressure environment is desired. Off-nominal

situations can also arise in which lower pressure/higher oxygen concentration environments need to be considered. Some examples may include vehicle leak emergency scenarios or decompression times before an EVA. In all these cases, understanding how existing flammability data can be correlated to other environments would prove useful. In doing so, care should be taken, as the relationships between material flammability with oxygen concentration and partial pressure are complex. These relationships will be examined in the following sections.

Test Method and Environmental Conditions: NASA STD-6001 Test 1 Maximum Oxygen Concentration Self Extinguishment Thresholds

The test method used in this paper to examine flammability was the NASA STD- 6001 Upward Flame Propagation Flammability Test 1 [2]. Materials slated for use in space vehicles are required to undergo this test to evaluate a material's ability to self-extinguish in less than 15 cm (6 in.) as well as to establish its propensity to propagate to nearby materials. Samples (12 in. long and 2.5 in. wide) are subjected to an overwhelming ignition source at their anticipated use conditions. After ignition, materials are evaluated to determine if they self-extinguish in less than 15 cm (6 in.), indicating that they are not likely to create sustained fires at the given test conditions. Also, paper is placed below the test apparatus during the test to evaluate if any dripping material will ignite nearby materials, thereby to evaluate a material's propagation risk. The Maximum Oxygen Concentration (MOC) threshold, as the name suggests, establishes the MOC for which a material will still pass the test pass/fail criteria. This threshold value can be used successfully to compare materials performance across various conditions [3, 4]. The MOCs for various aerospace materials have been previously determined across a large range of pressures (2.8–119.3 kPa (0.4–17.3 psia)) [5, 6, 7]. Much of these preexisting data have been compiled in Table 2 to allow a comprehensive analysis with respect to the effect of oxygen concentration, total pressure, and partial pressure on overall self-extinguishing limits. From MOC limits, the corresponding oxygen partial pressure limits were also calculated as Maximum Oxygen Partial pressure (MOP). The MOPs presented at 6.2 kPa (0.9 psia) or below, however, were determined experimentally in a 99.8% oxygen environment

where pressure was increased until the threshold limit was obtained at which materials still passed NASA-STD-6001 burn length criteria [7].

Oxygen Concentration, Total Pressure, and Partial Pressure Effects Findings

Oxygen Concentration and Total Pressure Findings

Maximum oxygen concentration data from Table 2 were plotted against total pressure in the 48.3–119.3 kPa (7–17.3 psia) range in Figure 1. Pressure data below 7 kPa (1 psia) were not plotted in Figure 1, as only five of the 22 materials examined had data in this lower range. This plot can be used to observe general effects of total pressure on MOC. Each material data set was fit with the equation that provided the highest regression analysis coefficient of determination (R^2). In the 48.3–119.3 kPa (7–17.3 psia) pressure range, most materials were best described by either linear or power curve models. Also, normoxic equivalent oxygen concentrations, all equaling a partial pressure of 21.3 kPa (3.09 psia) at their respective set of conditions, were plotted with red stars and corresponding curve. Normoxic data provide a comparison to the trends seen for the experimental flammability data for the various aerospace materials. Seventeen of the 22 materials examined (77% of materials) exhibited very little dependence on total pressure. For these 17 materials in the central pressure range of 48.3–119.3 kPa (7–17.3 psia), MOC remained relatively constant despite pressure variations. The general slope of the normoxic equivalent oxygen concentrations follows a steep decline while the general slopes of the tested materials' MOCs follow significantly shallower paths.

It is noteworthy that this contrasting trend from partial pressure dependent normoxic conditions to the experimental material data suggests that propagation and self-extinguishment flammability is not driven by the partial pressure of oxygen available. Oxygen concentration appears to be the major driver in propagation and self-extinguishment behavior regardless of total pressure or partial pressure of oxygen.

Other relevant research reiterates these conclusions. These include flame spread rate testing that was performed along normoxic conditions from 18% to 100% O₂ by Olson and Miller [8]. In this work, regardless of test variable modifications, the flame spread rate increased with higher oxygen concentrations even though partial pressure of oxygen remained constant [8]. In addition, authors Yang, Hamins, and Donneley [9] found that burn rates of poly(methyl methacrylate) (PMMA) spheres increased significantly as O₂ % volume was increased from 19.9% to 30% while little effect was observed with increased pressures from 50.0–150 kPa (7.25–21.75 psia) .

Though not fully modeling normoxic partial pressure trends, a few of the materials tested for this study (Kel-F^{®1}, polytetrafluoroethene (PTFE), Zotek^{®2} F30, Armalon TG4060, and Nomex^{®3}) exhibited higher dependencies on total pressure. A possible theory to explain the oxygen concentration and pressure dependence difference between these materials will be discussed in a later section.

In Figure 2, MOC self-extinguishment thresholds were again plotted against pressure with the inclusion of threshold pressures obtained at 99.8 volume% oxygen for select materials [7]. These material data sets with larger data ranges were again fit with equation models that provided the highest regression analysis coefficient of determination (R²). Power equation models fit all trends very precisely. It is believed that if additional high oxygen concentration data are obtained for other materials, they will likely show similar power trends. Flammability trends found here echo trends seen in previous ignition studies by authors Nakamura and Aoki [10, 11, 12], with the exception that a non-ignition zone is not identified in the current study. From this larger range view of flammability performance, it was again shown that total pressure had a minimal effect on propagation and self-extinguishment above approximately 41 kPa (6 psia). Nonetheless, below 41 kPa (6 psia) the pressure effects became highly influential. It has been proposed that different ignition models govern ignition mechanics in these two zones, with the pure

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² Zotek[®] is a registered trademark of Zotefoams PLC, Surry, U.K.

³ Nomex[®] s a registered trademark of E.I. Du Pont de Nemours and Company, Wilmington, DE.

diffusion model governing in the 48.3–119.3 kPa (7–17.3 psia) range and the ignition in stagnation-point flow field governing in the < 41 kPa (< 6 psia) range [13]. These proposed differing models for middle and low pressure ignition and propagation would be consistent with the findings drawn from Figure 2 and the corresponding data set.

Oxygen Partial Pressure Findings

From MOC testing, equivalent MOP pressures were calculated (presented in Table 2). The MOP represents the threshold value for how much oxygen is necessary to propagate a flame yet self-extinguish within the NASA-STD-6001 15 cm (6 in.) burn length criterion. MOP data were plotted against total pressure in Figure 3 to examine partial pressure effects directly. The clearest observation is that the required partial pressure of oxygen necessary to sustain propagation to the 15 cm (6-in.) criterion decreases with decreasing total pressure for all 22 materials examined. Therefore, despite having equal partial pressures, a lower pressure/higher oxygen concentration environment would pose a greater flammability risk. These findings are consistent with partial pressure ignition data trends observed by authors Nakamura and Aoki in which partial pressure of oxygen required for ignition of cellulose material decreased as total pressure was decreased [10, 11, 12].

Equations were fit to data for materials possessing full-scale pressure data. Power equation models described the data excellently with all coefficient of determination (R^2) calculated at higher than 0.99 values. It is believed that if additional data are obtained for other materials in the low pressure/high oxygen concentration ranges, they will likely show similar power trends.

With respect to how to apply existing data to alternate environmental conditions, the conclusion drawn from these data is that lower oxygen concentration/higher pressure data (e.g., 21% O₂, 101.4 kPa (14.7 psia)) cannot be conservatively applied to higher oxygen concentration/lower pressure environments

(e.g., 30%, 70.3 kPa (10.2 psia)) despite equivalent partial pressures. Nonetheless, higher oxygen concentration/lower pressure data (e.g., 30%, 70.3 kPa (10.2 psia)) can be conservatively applied to evaluate the risk of lower oxygen concentration/higher pressure environments (e.g., 21% O₂, 101.4 kPa (14.7 psia)).

Discussion: Oxygen Molecular Collision Rate Competition for Reaction Sites

Oxygen molecular collision rate competition for reaction sites is proposed as a potential theory to help describe the reported experimental trends. The major trends observed in examination of data are as follows: Oxygen concentration is the major driver for material flammability with little effect from total pressure in standard pressure ranges above 41 kPa (6 psia); decreasing amount of oxygen partial pressures are needed to support propagation as total pressure is decreased; and certain materials such as Kel-F, PTFE, Zotek F30, Armalon TG4060, and Nomex exhibited higher flammability pressure dependencies than other materials.

Piloted ignition and combustion of a material are normally described as a series of three events: a material heating time resulting in pyrolysis with corresponding generation of flammable gasses; an oxidizer and flammable gas mixing time; and an induction or chemistry time [14]. Nonetheless, in trying to not only explain rationale behind oxygen concentration as a primary flammability driver but also the rationale behind why certain classes of materials might exhibit different dependencies on pressure, an additional step may be proposed—one where the oxygen molecular collision rate competition for available reaction sites may play a role.

At two different conditions along the normoxic curve, partial pressure of oxygen and a therefore equivalent quantity of oxygen molecules are available. Nonetheless, the normoxic point that resides at the higher oxygen concentration and lower total pressure possesses a smaller percentage of inert molecules.

In the test environment, molecules are continually colliding with the material surface. Conditions with increased percentages of oxygen offer a higher chance of an oxidizer molecule coming into contact with a reaction site versus the corresponding normoxic condition with fewer competing inert molecules. This would explain why increased oxygen concentration escalates flammability despite equivalent partial pressures of oxygen. The same rationale holds true for the observation that decreasing amounts of oxygen partial pressures are needed to support propagation as total pressure is decreased. Decreased total pressure means less molecules as a whole competing for reaction sites. With decreased competition from inert molecules, it would make sense that less oxygen molecules are necessary to maintain similar flammability performance.

Recall that the materials exhibiting higher flammability pressure dependencies were Kel-F, PTFE, Zotek F30, Armalon TG4060, and Nomex. All of these more highly pressure dependent materials are highly halogenated, with the exception of Nomex. Kel-F is a thermoplastic chlorofluoropolymer, polychlorotrifluoroethylene (PCTFE), with the molecular formula $(CF_2CClF)_n$. Polytetrafluoroethylene (PTFE) is a fluoropolymer such as Teflon^{®1} with the molecular formula $(C_2F_4)_n$. Zotek F is a closed cell polyvinylidene fluoride (PVDF) based foam with the molecular formula $(C_2H_2F_2)_n$. Armalon TF 4060 is a fluorocarbon fiberglass composite. Because of their saturated chains of highly electronegative halogenated molecules (F, Cl), these materials are highly stable and possess few susceptible reaction sites. Though Nomex is not a halogenated compound, its aramid structure provides a highly stable structure with dense electron clouds that also offer few susceptible reaction sites.

If reaction sites are eliminated from the ignition initiation equation, then the oxygen molecule collision rate competition for reaction sites may no longer play a significant role as proposed earlier. Therefore, a material may directly follow the pyrolysis, mixing, and induction ignition model without an additional

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oxidizer reaction site collision rate accelerating step [14]. In these cases, a material may exhibit a higher pressure dependency (as was seen for Kel-F, PTFE, Zotek F30, Armalon TG4060, and Nomex) than what was seen for its more reaction site rich material counterparts.

The proposal that an oxygen molecule reaction site collision rate competition step may supplement the ignition sequence of pyrolysis, flammable gas mixing, and ignition induction appears to be successful in describing reported experimental trends.

Conclusions

The desire to understand how to apply existing enriched oxygen environment flammability data to alternate environmental conditions arises for NASA, commercial space flight companies, and industry alike. The question as to whether data can be applied to alternate environments based on partial pressure equivalents comes up frequently. Existing data from various sources have been compiled and examined here to address this common question. Analysis of data generated a series of observations. Flammability characteristics (per NASA-STD-6001 Test 1 MOC self-extinguishment thresholds, material ignition, and burn rates) show a strong dependence on oxygen concentration with little relation to total pressures above 41 kPa (6 psia). Below 41 kPa (6 psia), MOCs and required oxygen partial pressures show increased dependence on total pressure. Power equation models fit trends very precisely across pressure ranges spanning 2.8–119.3 kPa (0.4–17.3 psia) for both MOC and partial pressure plots against total pressures. A notable finding was that required partial pressure of oxygen necessary to sustain propagation decreases with decreased total pressures. This directly implies an increased flammability risk at lower total pressure conditions. This method of analysis may aid in the application of existing flammability data to alternate environmental conditions, and may ultimately provide guidance as to the types of tests that should be performed to yield the most useful results.

The conclusion drawn from these data is that lower concentration/higher pressure data (e.g., 21% O₂, 101.4 kPa (14.7 psia)) cannot be conservatively applied to higher oxygen concentration/lower pressure environments (e.g., 30%, 70.3 kPa (10.2 psia)) despite equivalent partial pressures. Nonetheless, higher oxygen concentration/lower pressure data (e.g., 30%, 70.3 kPa (10.2 psia)) can be conservatively applied to evaluate the risk of lower concentration higher pressure environments (e.g., 21% O₂, 101.4 kPa (14.7 psia)).

Certain materials (Kel-F, PTFE, Zotek F30, Armalon TG4060, and Nomex) exhibited higher dependencies on total pressure and are believed to perform differently due to their limited amount of susceptible reaction sites. A step for oxygen molecular collision rate competition for reaction sites was suggested as an additional mechanism in the ignition sequence of pyrolysis, flammable gas mixing, and ignition induction. This mechanism appears to be successful in describing reported experimental trends. Future planned work includes additional testing in low pressure ranges as well as acquisition of burn rate data of the presented materials at the various normoxic conditions.

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Table 2—Pressure effects on NASA STD-6001 Test 1 MOC flammability thresholds of materials for aerospace applications and equivalent normoxic and ISS environment conditions for comparison.

Material	psia (total pressure)													
	Determined at 99.8 % volume O ₂													
	0.4	0.5	0.6	0.9	7	10.2	12.35	14.7	17.3					
MOP (psia)	MOP (psia)	MOP (psia)	MOP (psia)	MOC (vol%)	MOP (psia)	MOC (vol%)	MOP (psia)	MOC (vol%)	MOP (psia)	MOC (vol%)	MOP (psia)	MOC (vol%)	MOP (psia)	MOC (psia)
PTFE					53	3.7			46	5.7	42	6.2		
KelF-81					76	5.3			56	6.9	53	7.8		
Silicone					28	2.0			23	2.8	21	3.1		
Zytel 42					25	1.8			23	2.8	23	3.4		
Viton-A					29	2.0			21	2.6	21	3.1		
Buna-S					18	1.3			17	2.1	16	2.4		
Neoprene					18	1.3			17	2.1	16	2.4		
Buna-N					18	1.3			16	2.0	15	2.2		
EPDM Rubber					18	1.3			16	2.0	16	2.4		
Polyethylene (PE)					18	1.3			18	2.2	17	2.5		
Delrin					13	0.9			12	1.5	11	1.6		
Zotek F30					47	3.3					37.5	5.5	36	6.2
Valox DR48					31	2.2					28.1	4.1	28	4.8
Nylon/ Phenolic					18	1.3					17	2.5	17	2.9
Armalon TG4060					50	3.5					35	5.1	33	5.7
Sygef							34	3.5			34	5.0	32	5.5
Udel P1700														
Polysulfone				0.9			29	3.0			24	3.5	22	3.8
Ultem 1000				0.9			24	2.4			21	3.1	21	3.6
Melamine/ Glass							36	3.7			34	5.0	33	5.7
Melindex 515	0.4						20	2.0			18.5	2.7		
Kydex 100				0.6			32	3.3			32	4.7	28	4.8
Nomex 90-40			0.5				37	3.8			31.5	4.6	30	5.2
Normoxic environment partial pressure equivalents (CEV/STS)					44	3.1	30	3.1	25	3.1	21	3.1	18	3.1
ISS environment partial pressure equivalents					50	3.5	34	3.5	28	3.5	24.1	3.5	20	3.5

MOC = Maximum oxygen concentration which consistently results in material self-extinguishment

MOP = Maximum oxygen partial pressure when extinguishment occurs (based on MOC with the exception of 99.8% testing)

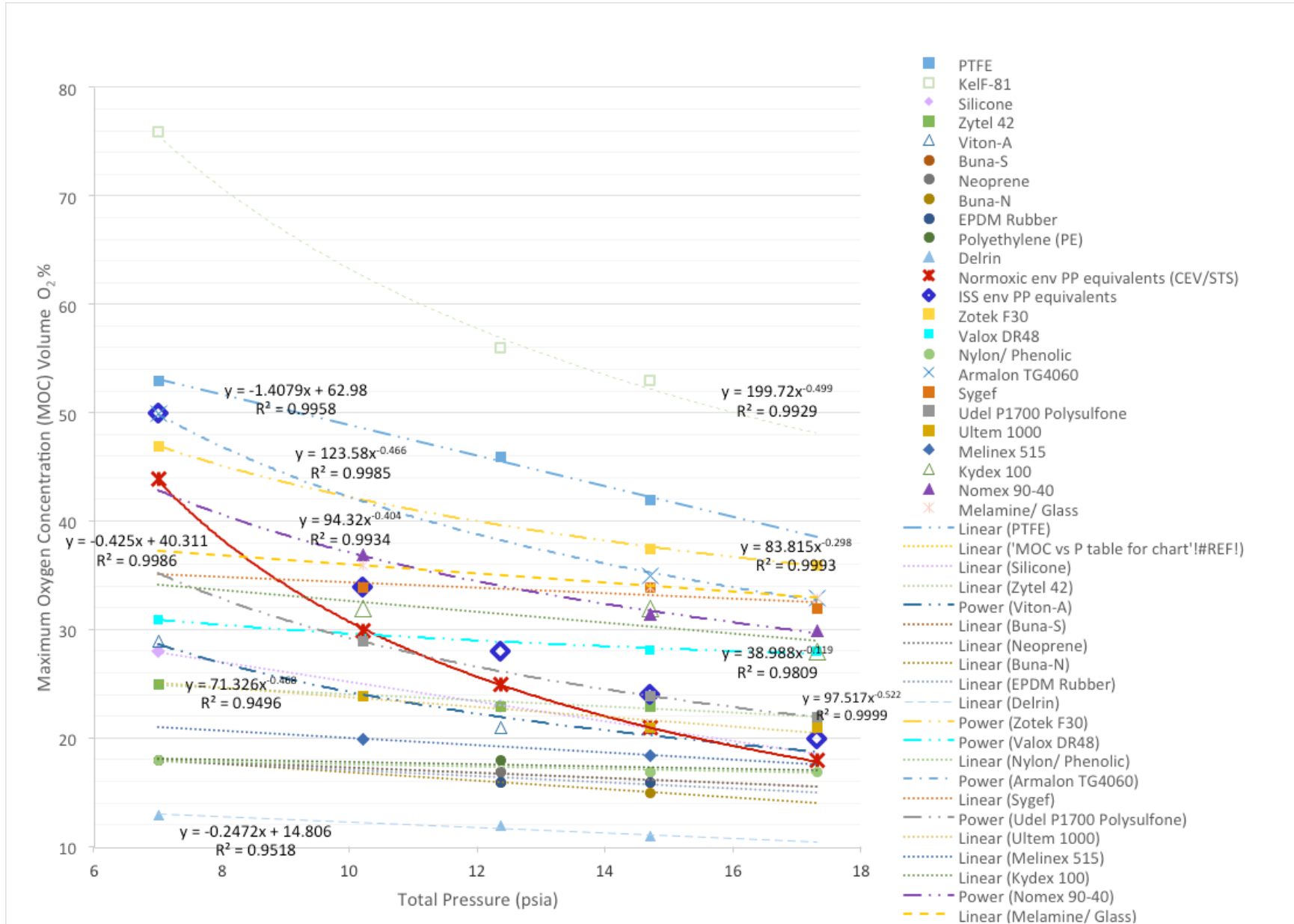


FIG. 1—Pressure effects on NASA STD-6001 Test 1 MOC flammability thresholds.

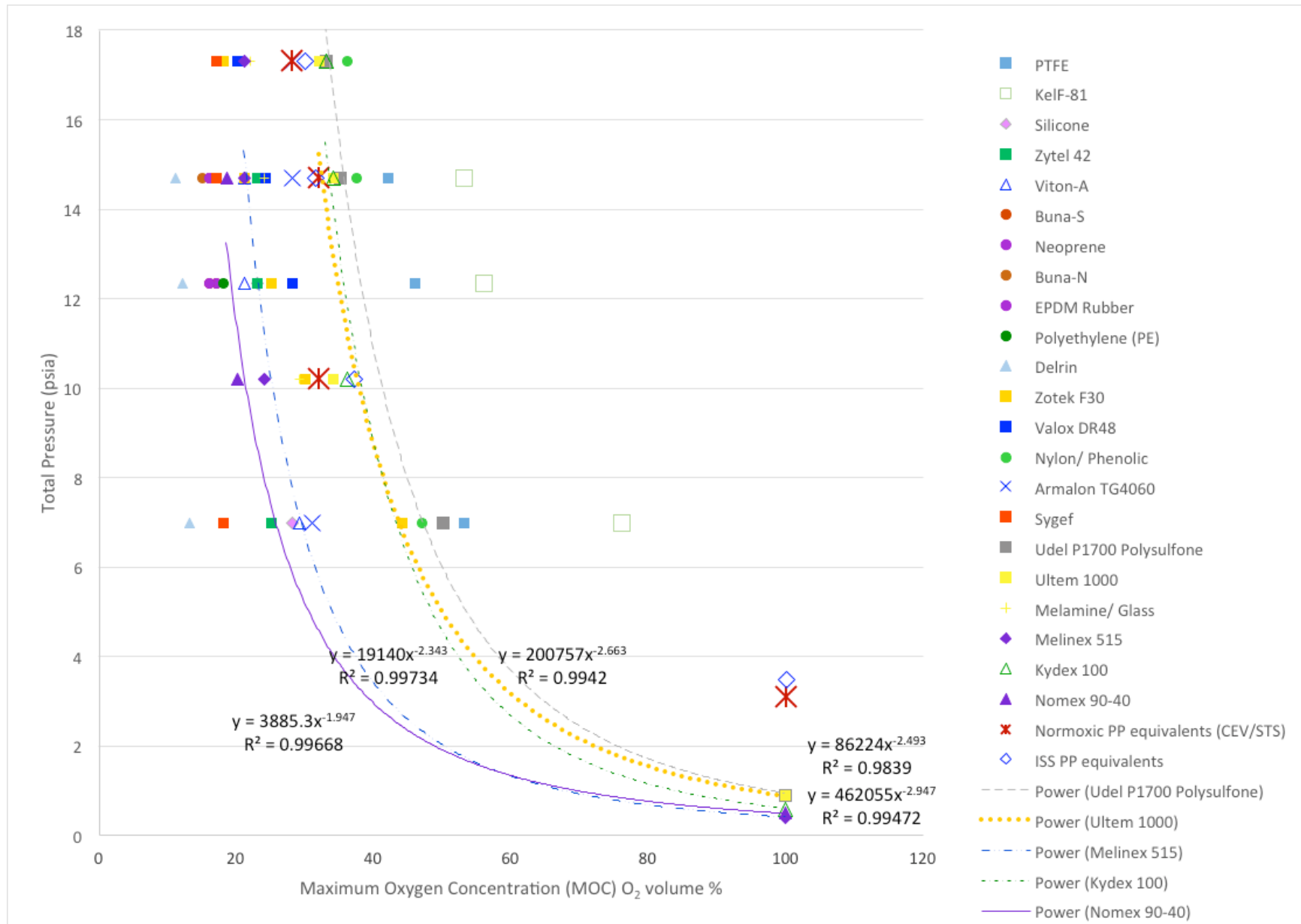


FIG. 2—MOC threshold in which NASA-STD-6001 Test 1 will consistently self extinguish, and equivalent normoxic oxygen concentrations.

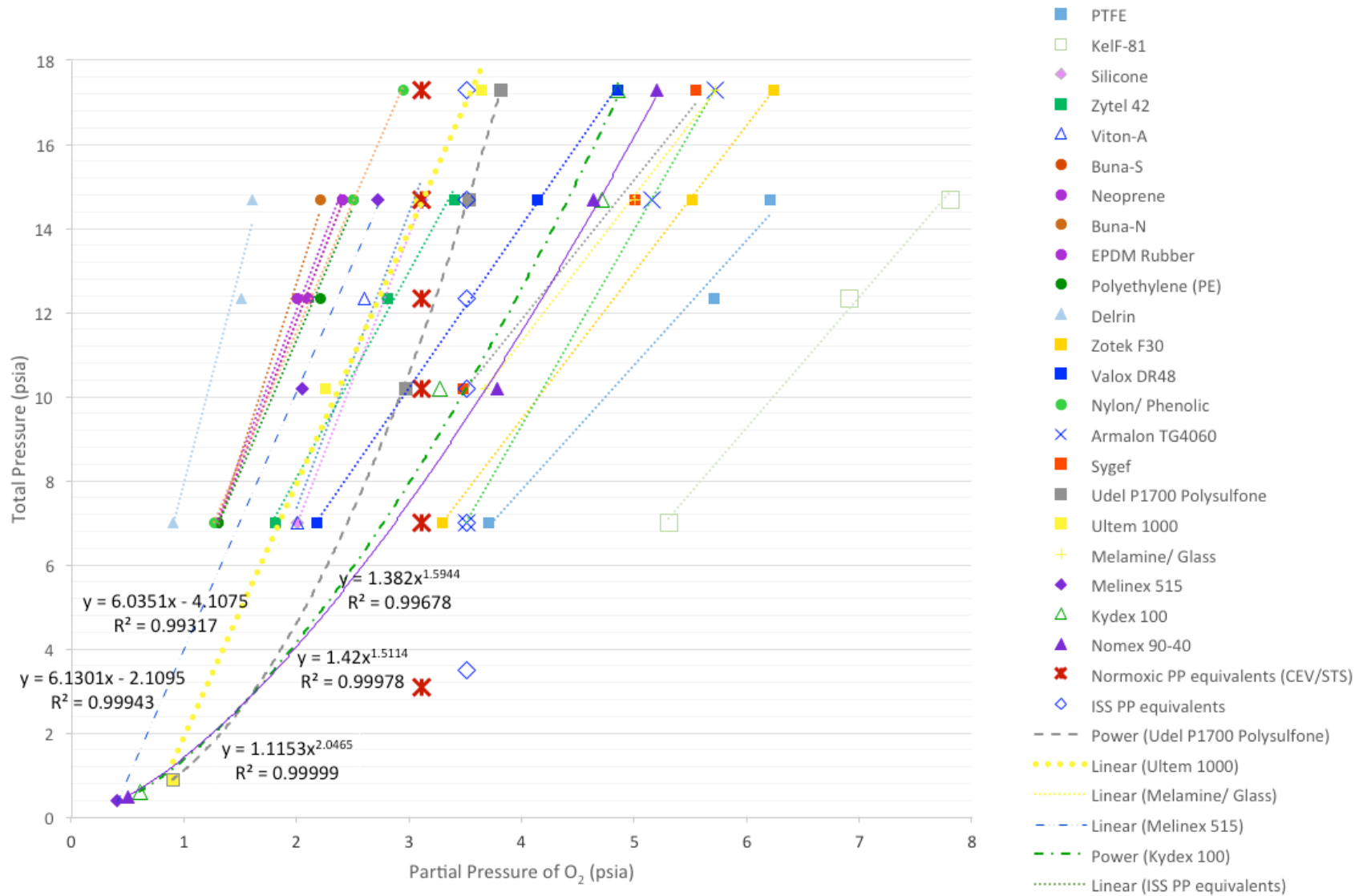


FIG. 3—MOP thresholds in which NASA-STD-6001 Flammability Test 1 will consistently self extinguish, and equivalent normoxic partial pressures.