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Standards for Computer Algorithms for Oxygen System Safety Analysis

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ABSTRACT: Computer software can provide support and serve as a double check on numerous calculations used in assessing materials fire risks in oxygen. However, software can be misused and its results may seem more credible than prudent. A draft proposed standard addresses five commercial, free and/or prototype algorithms and provides results and precautions that can help ensure results produced are consistent with prudent, skilful and practical use.

KEY WORDS: Computer algorithms, G4Math, O2Math, Computational Fluid Dynamics, Thermo-physical Properties, Thermo-Chemical Equilibrium

Computer software that substitutes for human labor and even intelligence (the latest called “artificial intelligence”) has become ubiquitous for facilitating all kinds of tasks. However, software for oxygen system safety analysis is not among the most common kind. Nor are the needs of oxygen systems safety analysis either routine or simple. The ASTM G4 collegium has numerous instances in which calculations were performed incorrectly and published, in which software was flawed or misused, in which the mathematics of an analysis were discouragingly onerous or otherwise too-daunting to undertake and where the software was otherwise misused. In every case the hazard of oxidant use can be increased. Targeted, carefully-used software can improve this oxidant safety pursuit and has improved it, even if artificial intelligence threatens to soon take away concerns for human limitations or even as some fear, needs for those humans to exist.

In 1992, ASTM G4 launched a series of computer “utilities” to assist the oxygen safety collegium which included highly trained academics (who nonetheless were not and are still not immune from these issues) ranging all the way to front-line rank-and-file oxygen users who have little or no familiarity with the oxygen compatibility subject and its science, much less the applied math or even just the plain old four-function math. The utilities were distributed on diskette and later a CDrom and as a free download to the Committee, community and to the students of its Standards Technology Training (STT later Technical and Professional Training, TPT) course as a learning tool and for “spit-balling” aid but were disclaimed as “As Is” and “Use at Your Own Risk”. They were hence not a substitute for normal diligence but a possible double check on one’s own math adventures. Balloting improved their robustness for use. Over a period of about fifteen years, no bugs were found.

There have been a number of other software categories, both proposed prototype and commercial, that have been cited in the subject literature, and some of their topics specifically like Computational Fluid Dynamics, Thermo-Physical Properties and Thermo-

¹ No mailing address.

Chemical Equilibria (TCE) are virtually intractable to most workers without software.

In the mid-2000s ASTM opposed the distribution of G4's software (notwithstanding its ongoing marketing of a rather involved software program, CHETAH, for decades that may not have been as fully disclaimed). They argued that software lends too much credibility to its results and if ever proven wrong can pose a liability risk. These same criticisms can be applied to standards, including ASTM standards, and every defense of standards can equally be applied to vetted, balloted, voluntary-use software, especially since standards of recent decades have less claim to being "full consensus". G4 did not push back and submissively ceased distribution of its utility ostensibly for that main reason but also potentially for less compelling reasons. To wit: the 16-bit software was also becoming obsolete to use on the latest 64 bit computers. It could have been easily upgraded but G4 apparently lacked the stomach for that. In this judgment G4 was in the midst of a wider slide into a darker less relevant age.

However, the mere fact that ASTM beseeched G4 not to provide software is highly suggestive that G4 could have done so if it truly wanted to. G4's capitulation is again suggestive of what at that time was a general withdrawal away from full-consensus products to a more exclusive narrower community. Furthermore while there is a form of equivalence between "a printed standard that suggests use of a material based upon data in a Table in the Standard" that is not that much different than suggesting "use based upon the results of the software that generated the table", but there is also that intangible smoke-and-mirrors difference. Hence while G4's cognoscente may consider software too risky, or too much work to prepare and distribute or even of insufficient benefit to pursue, or may have still other less "compelling" reasons, it has *not* taken a position to discourage the use of software as unhelpful or even antithetical to G4's mission. G4 and the oxygen safety community use numerous softwares in its operations to generate data and material for its standards and in papers published in its symposium series and seminar series. And in fact, sometimes the results have appeared to contain error.

However, Committee G4's mission (e.g. to save lives, injuries, capital and production) leads G4 to boldly publish data (that may be flawed) for example regarding the comparative benefit of assorted metals and their alloys. This is specifically because it is feared that, in at least some applications, use of some metals like aluminum instead of a metal like copper would less well serve to enhance safety and might demand special precautions.

Similarly, G4 can and should take stands, albeit "consensus" stands with thorough context for voluntary use. Consensus standards are by their very nature opinions that take stands even if those stands are disclaimed. as to related risks or exceptional cases. As voluntary standards, G4's products are inherently "as is" "use at your own risk" and standards on the use of software, even without distributing the software are as prudent as standards on how to clean hardware, or standards that cite authoritative references, especially since there is the stipulated concern that software decisions can effect oxygen system safety. It is dereliction to flag the hazards of use or misuse of one material over another and yet not flag the hazards of use or misuse of one algorithm over another. Data published in ASTM standards does not spring ex-nihilo, it is developed, it is measured, it is calculated, and quite often it is extracted from software or ad-hoc research. And soon that artificial intelligence issue will complicate things even more (even as ASTM disdains its use²).

²ASTM currently warns against the use of AI software on its website.

As a result, this is to argue that while G4 can abandon the benefits and needs for software creation and distribution (something that is counter to and does *not* advance its mission), the potential resulting negative consequences detract from the mission it claims to serve. However, like standards for the use of any lab instrument, standards on software and its uses are precisely within G4's wheelhouse/bailiwick.

Among the most urgent categories that G4 should address are (1) its own public domain algorithm that has been formerly vetted, balloted and distributed, (2) thermo-physical properties software, (3) computational fluid dynamics software, and perhaps most challenging and yet most needed (4) thermo-chemical equilibrium software (this latter case the further subject of a separate proposed standard on certain data it can estimate).

However, until artificial intelligence renders us all infallible (and unnecessary), software use, like oxidant use itself, is not without challenges. Not only is some software unable to deal with some situations, its extreme complexity can lead to or magnify misuse even where its use is otherwise valid, and the assorted software that is vital to exploit today's theory, has exhibited bugs and quirks that one must be wary of, and finally there have been mechanisms in nature that thwart perfect analysis and that need flagging, with or without software in the picture. Finally in some cases, for all the cited categories of data: software, tables, figures and conclusions, typical example situations should be generated and published as exemplars and calibration to help users avoid making the same kinds of errors and identify bugs or corruptions of their hardware that have plagued oxidant users and G4 itself in the past.

As a result, the included appendix proposes first draft context and suggestions (voluntary "as is" and "use at your own risk") for software use as a starting point for any committees including G4, a task group, or even just a social discussion group on software function. This is not a committee originated nor endorsed draft, but it employs a similar format of a standard not unlike those that ASTM, NFPA, ASME, etc. publish.

Context and Conclusion

Oxidant safety is a nontrivial subject. When confronted, the hazards of oxidants have resulted in loss of production (in some cases on a cubic-money scale), loss of capital (also in some cases on a cubic-money scale), and worst of all both gruesome injury and loss of life sometimes on a multiple scale.

Those writing safety standards and also safety regulations often face harsh choices. Among them can be decisions about whom to save. For example, several times in the 1980s/90s The National Highway Traffic Safety Administration regulations altered safety hardware (safety belts) in a way intended to entice their use by making them easier-to-use and therefore more likely to-be-used to save greater numbers of lives among the large group of safety-negligent drivers who did not wear safety belts. However, at the same time, the changes reduced safety-belt effectiveness among the most safety conscious and diligent users increasing the risk and doubtless number of deaths in that smaller group. Oxidant standards and software use present a similar dichotomy that is best avoided by making all options available for *voluntary* use.

Voluntary safety group's like ASTM G4, do not face this same dilemma. Voluntary

standards, can and should cite all options and the various known benefits and detriments of each. It is not, at present, G4's place to make decisions for anyone but themselves. However, it would be dereliction in this view to withhold known options, even disputed options, with suitable cautions and full disclosure.

Such is within the ability of G4 to do, and in its standards, including in standards that review and comment on software, and yes, including in software that it is able to produce and distribute. While censoring software on the implied basis that G4 lacks the skill or even worse the will and desire to prudently provide context might reduce liability fear, whether the fear is realistic, significant or not, the bottom line is that fewer lives will be saved, fewer gruesome injuries will be prevented, less capital will be saved, and less mission will be maintained. And to this commentator those are breeches of the G4 mission.

NOTE: *This is not an ASTM Standard, nor standard draft, but rather a shadow-standard proposal for a standard that hopefully someday can aid in the adoption of such a standard. This approach seeks to specify a data format that can be published and matured with suitable vetting. It does not seek to address flaws and shortcomings that are possible, but rather suggests the resources and data shown here that may be valid. Users are welcome to consider this opinion and factor it into their decisions in the same way that they consider the voluntary standards issued by ASTM Committee G4.*

Appendix

Proposed Format for a *Guide for the Use of Computer Algorithms for Oxygen System Safety Analysis*

1. Scope—Among the materials used to cope with fires and explosions in oxygen system are past incidents, experimental results, and theoretical interpretations. All of these may be dependent upon mathematically intense analyses. This guide applies to the use of selected and appraised computer software applications designed and intended to make these analyses more realistic and accurate and less onerous and prone to error. Such software may be routine and robust but may also be esoteric and obscure and so this guide seeks a consensus context for their use and limitations.

2. Referenced Documents—To Be Decided (TBD)

3. Proposed Terminology

3.1 Proposed Definitions – TBD

3.2 Proposed Description of Terms Specific to This Standard – TBD

4. Significance and Use—Among specialized computer software categories and implementations that can address oxygen system hazards, material selection, incident analysis and design features are the following:

4.1 *G4Math12.exe*—legacy code developed for G4 to perform a series of calculations of parameters such as are detailed in G4 standards or that appear within the G4 Symposia or seminar series. Noncommercial.

4.2 *O2Mathxx.exe*—a draft upgrade of G4Math12 to run on 64-bit Windows PCs based upon newer revisions of its resource materials. Not distributed as of this writing. Noncommercial.

Draft Proposal—04/27/26

Not vetted for use.

4.3 *FLLAME (Fire Limits for Linear-Afflicted Minds Everywhere)*: a proposed algorithm for coping with ternary (possibly future quaternary) diagram fire-limit interpretation that G4 declined to refine. Draft noncommercial copies were available in the 2000s.

4.4 *NIST Thermo-Physical Properties Database (free and commercial versions)*.

4.5 *Computational Fluid Dynamics (CFD) software (Fluent, CF-5, TOPAZ)*— cited in a small number of G4 symposium papers and meeting discussions. Some commercial, some unavailable.

4.6 *Thermo-Chemical Equilibrium calculation software (NASA Gordon-McBride, NASA Chemical Equilibrium for Applications, HSC Chemistry for Windows, FactSage)*— cited in numerous technical papers, controversial in some opinions and rejected for consideration within G4 by elements within its leadership. Some Free, some commercial.

4.7 *Specialized Reader Software*—another category of potentially useful software for some cases where data is presented in figures and curves where it is difficult to read and interpolate due to such things as logarithmic coordinate systems, axis units, and derivative calculations and conversions that may be desirable. This category and prototypes do not appear to have been effected nor discussed in G4 operations.

4.8 Each of these is qualitatively described, examples cited, and experience (benefits, limitations, and difficulties) are reviewed. These are not provided to represent recommendations which should ideally result instead from astute consideration. Note that ordinary non-oxygen-related software (so-called productivity word processor, spreadsheet, database, etc) are not addressed by this voluntary-use standard.

4.9 As is cautioned in ASTM and doubtless other standards, “the purpose of this standard is to furnish qualified technical personnel with pertinent information to use in selecting materials for oxygen service in order to minimize the probability of ignition and the risk of explosion or fire. It is intended for use in selecting materials for application in connection with the production, storage, transportation, distribution, or use of oxygen. It is not intended as a specification for approving materials for oxygen service”.

5. Consensus and Dissent—No draft standard such as this has been debated nor balloted and so a statement on consensus and dissent is not yet possible.

6. Issues Affecting Software Use

6.1 *Errors*. It is widely recognized that computer software has in the past generated results that while impressive and seemingly authoritative has nonetheless on occasion been wrong. Sometimes it has been wrong due to being used incorrectly. Sometime it has been wrong due to faulty software coding. Sometime it has been wrong due to its interpretation. This is not a unique issue. Graphs, charts, tables and standards themselves have also been wrong at times, as have been the extraction of data from them for these very same reasons. There is

no moral preference for one kind of error versus the other, however, in general, prudent algorithm use can result in a reduced rate of these errors. Such faulty data have found their way into other published standards and other resources. Hence just as it is common practice to include precision and bias commentaries in test method standards to cite what is possible to achieve, precision and bias statements are of no use when a standard or algorithm is misused. This standard seeks to not only recognize the potential benefits of software support but to also flag potential pitfalls in the use of pertinent software for oxygen safety use. It also seeks to provide vetted examples of results to use to learn and verify skillful use and appropriate coding.

6.2 Operational Obstacles. There are of course numerous hardware and installation issues that can be problems with all software. In some cases software does not run properly or at all. When obstacles are intractable, software becomes moot and users must fall back on the same abilities they would have to rely upon without software. However this is intended to comment on software that has ostensibly been correctly vetted, installed and is running correctly, but for which the underling mathematics is challenging for the non-routine user leading perhaps to acceptance of results without an intuitive feel for whether they are correct. Added to this can be software documentation that is daunting. As a result pertinent examples are included to train users and verify operations. But again when intractable, the user has his own skill set to employ.

6.3 Specialized Software

6.3.1 ASTM Committee G4MathXX.exe

6.3.1.1 Description: G4Mathxx is a Windows PC computer utility launched as a Version 1.0 in the early 1990s and revised to versions 1.1 and 1.2 (g4math10.exe, g4math11.exe, and g4math12.exe) during the 1990s. Written in Microsoft Visual Basic for Windows versions 1.0 through 3.0 (16 bit), it contains up to 4 screens each doing different calculations. Each version was balloted with no negative votes and within G4 there were general free mailings of diskettes with an installation system along with a series of other utilities and files. It was included with the G4 Standards Technology Training (STT) and later Technology and Professional Training (TPT) course and its operation was demonstrated therein through the 1990s, and somewhat later as well.

6.3.1.2 Distribution. In the early-to-mid- 2000s G4 ceased free distribution of the software. Nonetheless the endorsement for use was not terminated and existing instances may be running on legacy computer hardware. So-called support for the software ended, but there had been no need for bug-repair or revisions and the only glitch was in a download link that was inoperable and was fixed in the 90s. The only revisions were to add new functions/screens with each revision.

6.3.1.3 Software Nature: All early versions of G4Mathxx were a 16-bit software (MS Visual Basic 1.0-3.0) incompatible with newer 64-bit Windows PCs. The original code has

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Not vetted for use.

been upgraded to 32 bit (Visual Basic 4.0) as O2Math (see below) and can run on 64-bit Windows machines and may become available as free-ware. Both are on an “As is” and “Use at Your Risk” basis. Versions through G4Math12 have been balloted and distributed by G4. Specifically, its functions are cited below.

6.3.1.3.1 *Screen 1*. A tool for calculating adiabatic compression temperature and gas velocities in oxygen piping (along with values generated by CGA Pamphlet G4.4 circa 1990s)

6.3.1.3.2 *Screen 2*. A tool for calculating the suggested minimum test pressure for conducting the ASTM G 124-94 test.

6.3.1.3.3 *Screen 3*. A tool for calculating the sizes of Distance/Volume Pieces (DVPs) for use with polymer-lined flex hoses or similar applications (using equations derived in a paper by Santay et al. in *ASTM STP 1319 Flammability and Sensitivity of Materials in Oxygen-Enriched Atmospheres, Eighth Volume*, 1997).

6.3.1.3.4 *Screen 4*. A tool for calculating when bypass valves (for example single-use bypass valves) may not be necessary around isolation valves on the bases of (1) avoiding excessive adiabatic compression heating, and (2) avoiding excessive gas velocities within the isolation valve during opening (using equations derived in a paper by Castillo et al. in *ASTM STP 1319 Flammability and Sensitivity of Materials in Oxygen-Enriched Atmospheres, Eighth Volume*, 1997).

6.3.1.4 Experience—There were installation issues with downloaded copies of the earliest versions but no errors identified in the actual utility operations throughout its period of support (10+ years). Nor have G4 minutes cited lingering subsequent issues since the mid-2000s.

6.3.1.5 Reference Data—Appendices provide sample data generated with G4Math12 and believed correct (per the early experience and balloting of this standard) that can be used to test existing copies of either software package. These data may not be sufficient to establish suitability or adequate precision for any specific use and may be revised if needed.

6.3.1.6 Legacy Issues—Early G4Math12.exe software is still viable on legacy PC computers with 16-bit Windows OS and 32-bit Windows systems with 16 bit compatibility. It does not run on 64-bit PC computers with Windows OS, however software such as WineVDM or virtual machine installation is claimed to allow legacy 16-bit software to run. Neither Wine nor any virtual machine have been tested with any version of G4Mathxx.exe.

6.3.2 O2Math12.exe

6.3.2.1 Description: O2Math12.exe is a draft 32-bit Visual Basic 4.0 derivative capable of running in 32-bit Windows and in 64 bit Windows in its “compatibility layer”. It is based upon the same source code used for G4Math12.exe and upgraded. It has not been widely

distributed to date, vetted, balloted anywhere, nor has it developed any experience base. Conversion to alternative language (Python, VBNET) have been considered.

6.3.2.1 Distribution: O2Math12 has not been distributed. Its draft existence has been broached to ASTM G4 leadership, but no committee interest was present. Public domain or open source distribution remain possibilities.

6.3.2.3 Software Nature: As of this writing, O2Math contains the same four screens as G4MATH12 except that Screen 1 has been modified to incorporate calculation of CGA/EIGA revised gas velocities as revised in the 2000s. A glitch identified (two recommendations in the early standard for the same conditions was identified that may or may not still be present as of this writing). Tenuous prospects to add screens for simplistic TNT equivalence calculations, worst case adiabatic compression energy transfer scenarios, and perhaps software reader abilities for specific graphical data have been considered.

6.3.2.4 Experience: There is no experience base for O2MATH.

6.3.2.5 Reference Data—Reference data are the same as for the equivalent earlier G4Math12.exe version and are shown in the appendices that can be used to test existing copies of either software package. These data may not be sufficient to establish suitability or adequate precision for any specific use and may be revised if needed.

6.3.2.6 Legacy Issues—O2Math12.exe has not been made public as of 2026, but trial copies may be available for use with 32 bit PCs or 64 bit Windows that have a compatibility layer facility. Operation on Linux or Apple operating systems may be possible on Windows simulation or virtual machines.

6.3.3 FLLAME (Fire Limits for Linear-Afflicted Minds Everywhere)

6.3.3.1 Description: FLLAME.exe is an experimental software draft developed in a corporate environment to interpret fire-limits of flammable gas mixture graphical data using ternary diagram data and methods, typically found in U.S. Bureau of Mines publications. FLLAME has been released for development into a public utility. ASTM G4 considered a derivative effort in ~2000, however, ternary data were so despised for their complexity and ease of misuse and error that there was strong opposition to undertaking such effort, despite the promise software held to reduce such error. A commentary [I]¹ has been prepared to introduce the pertinent concepts of binary, ternary and even potential future quaternary analysis. A high-level leadership task force was created in ~2000 to study the options (but presumably “shelved” it as the Task Force has not been heard from since). Although a basis for opposition was that G4 only addresses structural materials, the argument was specious in that G4 addresses lubricants and diluents and other examples of “non-structural” materials. Indeed, a PC algorithm may present the best way to expand the use of these critical data while reducing the extreme chances of error. **FLLAME.exe** is a 16-bit Visual Basic 3.0 de-

¹Boldface italic numbers in brackets refer to the reference list at the document end.

rivative capable of running in 32-bit Windows but not 64 bit Windows. It has not been widely distributed to date (an early draft was available on a personal web site), vetted, balloted anywhere, nor developed any experience base. Its future is uncertain.

6.3.3.2 Distribution: FLLAME.exe has not been formally distributed. Draft copies were available in the 1990s for consideration.

6.3.3.3 Software Nature: As of this writing, FLLAME.exe is only a 16-bit draft that runs on 16 and 32 bit Windows systems that is suitable for development but has not been used for actual hazard analysis. A 32-bit revision is possible based on the original code but lack of interest may make that unlikely.

6.3.3.4 Experience: There is no experience base for FLLAME.exe. It has remained a proposed future prospect for more than two decades.

6.3.3.5 Reference Data—FLLAME addresses the extraction of data from experimentally established curves for up to three constituents. An appendix in this standard to exhibit example data may be a future addition.

6.3.3.6 Legacy Issues—FLLAME.exe has not been distributed for public use as of 2026.

6.3.4 NIST Thermo-Physical Properties Data (TPD)

6.3.4.1 Description—The United States National Institute of Standards and Technology (NIST) has published its TPD software system in two installable versions at nominal cost and a free version that can be run on the internet at the domain: WebBook.nist.gov. NIST TPD software allows the generation of data for heat capacity, latent heat, melting and boiling points, internal energy (useful in estimating some TNT equivalencies), entropy, enthalpy and other data. As of 2026, it has been used to extract data for at least one unvetted commentary on oxidant safety [2].

6.3.4.2 Distribution—Distribution data are not available, however, the NIST resources have been available for more than a decade.

6.3.4.3 Software Nature: Operations of the Internet WebBook version is traditional. Software was distributed as a Windows 32 bit resource on CDROM in the early 2000s. Two different codings were available that were similar and contained data for many materials in common but each had unique entries as well.

6.3.4.4 Experience: There are few if any citations of data from these softwares in the ASTM G4 forum (standards or symposium or seminar materials) that cite this resource, but the NIST reputation for credibility is not challenged.

6.3.4.5 Reference Data—The massive scope of this software thwarts efforts to present reference data in an appendix at present. Reference [2] used the software to explore several

scenarios but has not been vetted for accuracy. However, real-gas data were generated from numerous equations of state (for oxygen, fluorine, nitrogen-trifluoride, ozone, nitrous oxide) allow for extracting) for adiabatic compression temperatures, TNT equivalencies, heat capacities, latent heats, phase transition temperatures, and more.

6.3.4.6 Legacy Issues—Legacy issues, if any, may be present on the NIST website.

6.3.5 Computational Fluid Dynamics (CFD) Software

6.3.5.1 Description - CFD software uses massively complex math to solve complex equations (e.g. Navier-Stokes equation) to estimate fluid flow and heat transfer issues. The theory is challenging and the software is equally challenging to apply even for the most lettered users. Nonetheless it can suggest flow patterns in piping: such as dual-vortex flow cited in ASTM Standard G88, or incident analysis that may help explain causation or may suggest designs that should be preferred or avoided. Things like where particles may impact warranting use of impingement plates. CFD software is often used to generate graphical results not readily subject to calibration examples. As a result, CFD analysis and software use is best left to experienced oxygen safety practitioners and little use of it has been made in the past. However, a dedicated task force might well be able to identify numerous flow scenarios that would benefit oxygen system design if generated and published as an atlas of data. This might include the dual vortex scenario, flow through restrictions and obstructions, fluid impact behaviors. etc.

6.3.5.2 Distribution—CFD software is available in several commercial configurations (FLUENT, CF-5) that are expensive and complicated to use. Dedicated training is often needed.

6.3.5.3 Software Nature: CFD results are often in the form of flow diagrams. Gas pattern flow over aerodynamic structures is the typical product.

6.3.5.4 Experience: The at-large experience base for CFD software is substantial, but little or no experience base has developed in the joint oxidant safety community. Two examples are found in references [3,4].

6.3.5.5 Reference Data—Only a small number of papers have been presented in the ASTM G4 forum including [3,4].

6.3.5.6 Legacy Issues—None known due to small amount of use.

6.3.6 Thermo Chemical Equilibrium (TCE) Calculation Software

6.3.6.1 Description—Thermo-Chemical Equilibrium (TCE) theory is a challenging subject

and the use of software to extract TCE property data is equally challenging, perhaps left best to highly trained specialists in the field and vetted by experienced oxygen safety practitioners. However, in at least some cases, once extracted, vetted and flagged for aberrant behaviors, TCE data can be quite useful and even simple and straight-forward to apply to actual oxygen system evaluations. Its promise was simultaneously broached, endorsed and then quickly rejected in 1992 by several of ASTM G4's most lettered members at the time who first applied its use with great difficulty to understanding metals combustion in oxygen [5]. Later efforts to reinvigorate its use 2008 found a steep and long learning curve fraught with pitfalls and a stubborn resistance within ASTM G4 leadership to undertake its use. TCE analysis integrates a number of historically observed behaviors into a composite theory that can provide improved understanding of fire and explosion scenarios in some cases but due to complexity and in some cases flawed exploitation can also provide controversial data. TCE theory and its software can estimate: adiabatic combustion temperature for standard or nonstandard conditions, heat of combustion for standard and nonstandard conditions, heats of dissociation for standard and nonstandard conditions, and combustion thresholds ("burn ratios") for standard and nonstandard conditions.

6.3.6.2 Validity—Thermo-chemical equilibrium (TCE) behavior has a long history of use in numerous applications but scant history for oxygen system safety, and where used for oxygen system behavior, complexity, errors and confusion abound. Both the theory and software are well established for analyzing various chemical industry processes and for analyzing and remedying automobile and atmospheric pollution issues, and these established analyses are even more complex than the bulk of metals/oxygen combustion issues facing the oxygen safety community. Yet use in oxygen applications are few and there are valid reasons for that. All of these and other parameters can be daunting to generate and even extract from any of the software packages that are available (free NASA G-M code and commercial CEA for Applications, expensive commercial HSC Chemistry for Windows and FactSage). However, a group of simplified thermo-chemical "profiles" can be generated that warrants careful vetting and evaluation but which can be used by most, maybe all, for the entire range of oxygen safety practitioners. These profiles are much more useful than existing coarse tabulated data and may be approximate but could ultimately be expanded into an atlas of comparable data akin to the JANAF Tables of data upon which many TCE calculations are based. A separate stand-alone proposed standard of TCE thermal profile data generation and use has been prepared [6] and has been proposed.

6.3.6.3 Distribution: The NASA TCE software package is available for free at least since the 1990s and has been used by a core group to analyze rocket performance with a wide distribution. It was developed for rocket analysis, but it has been used only infrequently and with questionable facility for safe oxidant hardware use [5,7]. Outokompu introduced a Windows PC version of its HSC Chemistry program in the 1990s marketed largely for chemical process use but has been cited in few papers in the ASTM forum [8]. FactSage offers an apparently very powerful but also very expensive package. Indeed, several corporate proprietary systems are known to be in use but not available publicly nor cited in the open literature.

6.3.6.4 Software Nature: Thermo-Chemical equilibrium theory is a field of great complexity, and the software that helps cope with it is equally or more complex, too complex to briefly overview here. All implementations of TCE software appear to be extremely challenging not only to understand but to use, suggesting that derivative results be extracted and vetted by skillful panels of experts into an atlas for practical use [6]. Suffice it to say that TCE software is a mathematically intense activity with massive numbers of repetitive calculations and successive approximations.

6.3.6.5 Experience: There is no substantial experience base for TCE software in the oxidant safety community. It has been used in the ASTM Committee G4 community to generate thermo-physical property data [8] more so than combustion equilibria data. The few times it has been used to analyze combustion in oxygen, the results appear flawed, possibly misinterpreted, though interesting. It remains a curiosity and a future prospect of great but unharvested promise. Simplified derivative TCE data are however, employed commonly that have oftentimes been obtained not by theoretical estimates but by direct measurement.

6.3.6.5 Reference Data—While many data of the kind TCE software might predict are known, often due to direct measurement or approximate estimates, no consensus data are available for citing in appendices here as standard to use in checking user results. Example results would be possible if the community selected specific meaningful goals. Meanwhile only questionable results are present to check one's own results in several papers some of which are claimed to be in error and many are cited with tenuous conviction.

6.3.6.6 Legacy Issues—TCE software has no pertinent legacy at present in the oxidant safety community beyond initial endorsement, criticism and then discouragement. Some early software (NASA Gordon/McBride) was coded in Fortran IV and its demanding command line system led to apparent errors that appear to encumber opinions negatively to this day. A newer Windows front end may prove more accommodating at some point. Similarly, its focus on the high temperature combustion of rocket engines has made its use for oxidant system fire analysis even more difficult. Numerous tyro dabblings/efforts [9-13] have sought to understand, and adapt NASA and Outokumpu software to oxygen system safety use but are un-vetted, likely flawed, and have generated little-to-no interest in the community at large.

7. Practicality and Quality Issues—Some pertinent software (HSC for Windows) is not only practical but it yields data with fewer problems than NASA's CEA that can be checked to estimate accuracy and precision. Some software generates results that are not exactly reproducible even in repeat runs. Practicality and quality issues at present lack definition.

8. Precision and Bias—Although there are numerous numerical measures that can be determined with this theory and the resulting software, possible and necessary measures of precision and bias will need to be established by actual usage and so this must be considered a "provisional" draft standard proposal until it can be refined.

9. Correction, Evolution and Revision—As of this draft, TCE TCE theory and software

has had little exposure in the oxygen safety community. Its rather compelling learning curve awaits community interest. Similarly its use is too new for evolution and revision to be contemplated.

10. Keywords—TBD

11. References

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12. Appendices

12.1 Exemplar Data for G4Math and O2Math-TBD