Peer Review of Interim Report on Computational Fluid Dynamics Model for Predicting Wellhead Oil-Burning Efficiency at Bench and Intermediate Scales

Committee on the Peer Review of Interim Report on Computational Fluid Dynamics Model for Predicting Wellhead Oil-Burning Efficiency at Bench and Intermediate Scales

Board on Chemical Sciences and Technology

Division on Earth and Life Studies

A Consensus Study Report of
The National Academies of
SCIENCES · ENGINEERING · MEDICINE

Peer Review of Interim Report on Computational Fluid Dynamics Model for Predicting Wellhead Oil-Burning Efficiency at Bench and Intermediate Scales (2021)

DETAILS

52 pages | 8.5 x 11 | PDF
ISBN 978-0-309-68297-8 | DOI 10.17226/26211

CONTRIBUTORS

Committee on the Peer Review of Interim Report on Computational Fluid Dynamics Model for Predicting Wellhead Oil-Burning Efficiency at Bench and Intermediate Scales; Board on Chemical Sciences and Technology; Division on Earth and Life Studies; National Academies of Sciences, Engineering, and Medicine

SUGGESTED CITATION

National Academies of Sciences, Engineering, and Medicine 2021. *Peer Review of Interim Report on Computational Fluid Dynamics Model for Predicting Wellhead Oil-Burning Efficiency at Bench and Intermediate Scales*. Washington, DC: The National Academies Press. https://doi.org/10.17226/26211.

Peer Review of Interim Report on Computational Fluid Dynamics Model for Predicting Wellhead Oil-Burning Efficiency at Bench and Intermediate Scales

Committee on the Peer Review of Interim Report on Computational Fluid Dynamics Model for Predicting Wellhead Oil-Burning Efficiency at Bench and Intermediate Scales

Board on Chemical Sciences and Technology

Division on Earth and Life Studies

A Consensus Study Report of
The National Academies of
SCIENCES · ENGINEERING · MEDICINE

THE NATIONAL ACADEMIES PRESS
Washington, DC
www.nap.edu

THE NATIONAL ACADEMIES PRESS 500 Fifth Street, NW Washington, DC 20001

This activity was supported by contracts between the National Academy of Sciences and the U.S. Department of the Interior, Bureau of Safety and Environmental Enforcement (BSEE). This report has not been reviewed by BSEE, nor has it been approved for publication. Approval, when given, does not signify that the contents necessarily reflect the views and policies of the Bureau, nor does mention of the trade names or commercial products constitute endorsement or recommendation for use. Study concept, oversight, and funding were provided by the Department of the Interior, BSEE, Oil Spill Preparedness Division, Sterling, VA under OSRR Project 1063 Contract Number 140E0121C0002. Any opinions, findings, conclusions, or recommendations expressed in this publication do not necessarily reflect the views of any organization or agency that provided support for the project.

International Standard Book Number-13: 978-0-309-68297-8
International Standard Book Number-10: 0-309-68297-5
Digital Object Identifier: https://doi.org/10.17226/26211

Additional copies of this publication are available from the National Academies Press, 500 Fifth Street, NW, Keck 360, Washington, DC 20001; (800) 624-6242 or (202) 334-3313; http://www.nap.edu.

Printed in the United States of America

Suggested citation: National Academies of Sciences, Engineering, and Medicine. 2021. *Peer Review of Interim Report on Computational Fluid Dynamics Model for Predicting Wellhead Oil-Burning Efficiency at Bench and Intermediate Scales*. Washington, DC: The National Academies Press. https://doi.org/10.17226/26211.

The National Academies of
SCIENCES • ENGINEERING • MEDICINE

The **National Academy of Sciences** was established in 1863 by an Act of Congress, signed by President Lincoln, as a private, nongovernmental institution to advise the nation on issues related to science and technology. Members are elected by their peers for outstanding contributions to research. Dr. Marcia McNutt is president.

The **National Academy of Engineering** was established in 1964 under the charter of the National Academy of Sciences to bring the practices of engineering to advising the nation. Members are elected by their peers for extraordinary contributions to engineering. Dr. John L. Anderson is president.

The **National Academy of Medicine** (formerly the Institute of Medicine) was established in 1970 under the charter of the National Academy of Sciences to advise the nation on medical and health issues. Members are elected by their peers for distinguished contributions to medicine and health. Dr. Victor J. Dzau is president.

The three Academies work together as the **National Academies of Sciences, Engineering, and Medicine** to provide independent, objective analysis and advice to the nation and conduct other activities to solve complex problems and inform public policy decisions. The National Academies also encourage education and research, recognize outstanding contributions to knowledge, and increase public understanding in matters of science, engineering, and medicine.

Learn more about the National Academies of Sciences, Engineering, and Medicine at **www.nationalacademies.org**.

COMMITTEE ON THE PEER REVIEW OF INTERIM REPORT ON COMPUTATIONAL FLUID DYNAMICS MODEL FOR PREDICTING WELLHEAD OIL-BURNING EFFICIENCY AT BENCH AND INTERMEDIATE SCALES

Members

MARGARET WOOLDRIDGE (*Chair*), University of Michigan
JACQUELINE H. CHEN, NAE, Sandia National Laboratories
FREDERICK L. DRYER, NAE, University of South Carolina
TAREK ECHEKKI, North Carolina State University
IPSITA GUPTA, Louisiana State University
JOSEPH KATZ, NAE, The Johns Hopkins University
ROBERT P. LUCHT, Purdue University
HOPE A. MICHELSEN, University of Colorado Boulder
VEDHA NAYAGAM, Case Western Reserve University
ALI S. RANGWALA, Worcester Polytechnic Institute
ABHISHEK SAHA, University of California, San Diego
WILLIAM A. SIRIGNANO, NAE, University of California, Irvine
SIBENDU SOM, Argonne National Laboratory, University of Chicago

Staff

MAGGIE WALSER, Co-Study Director
LIANA VACCARI, Co-Study Director
JESSICA WOLFMAN, Research Associate
BENJAMIN ULRICH, Senior Program Assistant

BOARD ON CHEMICAL SCIENCES AND TECHNOLOGY

Co-Chairs

SCOTT COLLICK, DuPont
JENNIFER SINCLAIR CURTIS, University of California, Davis

Members

GERARD BAILLELY, Procter & Gamble
RUBEN G. CARBONELL, NAE, North Carolina State University
JOHN FORTNER, Yale School of Engineering and Applied Science
SAMUEL H. GELLMAN, NAS, University of Wisconsin–Madison
KAREN I. GOLDBERG, NAS, University of Pennsylvania
TIMOTHY HALL, McNesse State University
MIRIAM E. JOHN, Sandia National Laboratories (Ret.)
JODIE L. LUTKENHAUS, Texas A&M University
JOSEPH B. POWELL, Shell Global
SALY ROMERO-TORRES, Thermo Fisher Scientific
PETER ROSSKY, NAS, Rice University
REBECCA T. RUCK, Merck Process Research & Development
RICHMOND SARPONG, University of California, Berkeley
VIJAY SWARUP, ExxonMobil

Staff

JEREMY MATHIS, Board Director
MEGAN HARRIES, Program Officer
LIANA VACCARI, Program Officer
LINDA NHON, Associate Program Officer
NICHOLAS ROGERS, Senior Finance Business Partner
THANH NGUYEN, Financial Business Partner
KESIAH CLEMENT, Research Associate
JESSICA WOLFMAN, Research Associate
ELISE ZAIDI, Communications and Media Associate
ABIGAIL ULMAN, Research Assistant
BEN ULRICH, Senior Program Assistant
ANIA ZOLYNIAK, College Student Hire

Acknowledgment of Reviewers

This Consensus Study Report was reviewed in draft form by individuals chosen for their diverse perspectives and technical expertise. The purpose of this independent review is to provide candid and critical comments that will assist the National Academies of Sciences, Engineering, and Medicine in making each published report as sound as possible and to ensure that it meets the institutional standards for quality, objectivity, evidence, and responsiveness to the study charge. The review comments and draft manuscript remain confidential to protect the integrity of the deliberative process.

We thank the following individuals for their review of this report:

Laura DeMarco, NAS, Harvard University
Peyman Givi, University of Pittsburgh
Andrea Prosperetti, NAE, University of Houston
Kuochen Tsai, Shell
Krishna Venkatesan, GE Global Research
Yi Wang, FM Global

Although the reviewers listed above provided many constructive comments and suggestions, they were not asked to endorse the conclusions or recommendations of this report, nor did they see the final draft before its release. The review of this report was overseen by Dennis Bushnell, NASA, and Manuel Terranova, Peaxy, Inc. They were responsible for making certain that an independent examination of this report was carried out in accordance with the standards of the National Academies and that all review comments were carefully considered. Responsibility for the final content rests entirely with the authoring committee and the National Academies.

Table of Contents

APPENDIXES

Executive Summary

Wellhead combustion is an extraordinarily complex system involving an extremely large range both of scales and of physical hardware. Moreover, the diverse properties of crude oils and the different geographic settings of the wellheads (e.g., Arctic, off-shore) lead to significant challenges for developing predictive models of wellhead combustion. *OSRR 1063: Bureau of Safety and Environmental Enforcement Report: Computational Fluid Dynamics Model for Predicting Wellhead Oil-Burning Efficiency at Bench and Intermediate Scales: Interim Report* (July 30, 2020), produced by the U.S. Naval Research Laboratory (NRL) and funded by the Bureau of Safety and Environmental Enforcement (BSEE), includes summaries of computational modeling and experimental efforts to represent wellhead combustion toward the ambitious goal of predicting the combustion efficiency of wellhead flames. An ad hoc committee convened by the National Academies of Sciences, Engineering, and Medicine was charged with performing a peer review of this interim report encompassing the study methods, the quality of the data informing the study, and the strength of any inferences drawn by the NRL authors; accordingly, this final peer review report focuses on the technical nature of the interim NRL report (OSRR 1063).

The committee found that the authors performed foundational work for modeling and experimental research on some of the physicochemical mechanisms for physically downscaled wellbore processes. They identified some of the important aspects to be considered and developed some foundational understanding of physical and chemical processes relevant to wellbore ignition and combustion problems. They also summarized some relevant literature to provide context for their work. However, **the consensus conclusion of the committee is that the model developed is not adequate for predicting the combustion efficiency of wellhead flames**.

The major concerns identified by the committee through deliberation on the questions posed in its charge as provided by BSEE (Appendix A) can be divided into three general categories:

1. Gaps in the study approach and the assumptions chosen to represent the physical system of wellhead combustion limit the utility and accuracy of the approach and the model.
2. Several modeling approaches employed are not the state of the art.
3. Other modeling methods employed are the state of the art, but their related uncertainties and known weaknesses are not considered.

Regarding the utility of the approach and the assumptions applied in developing the model and its components, the wellhead system is not well defined, and the level of accuracy required or desired for the model is never identified. These are fundamental concerns that dictate which approaches for the modeling and experimental work—e.g., Reynolds-averaged Navier-Stokes (RANS) or Large Eddy Simulation (LES) modeling methods—are appropriate, or how crude properties are to be considered. Another key concern is the lack of well-defined initial and boundary conditions in the context of wellhead combustion.

Designing appropriate experiments with which to validate the model or help scale the results to actual wellhead combustion conditions is difficult without a well-defined problem. Without a well-defined problem, moreover, it is not possible to evaluate the adequacy of the model.

Other high-level technical findings as to the completeness of the modeling results for predicting wellhead oil-burning efficiency identified by the committee are as follows:

1. It is unclear whether the authors considered the correct flow system.
   a. Is the correct configuration for the multiphase flow considered? Specifically, is co-annular two-phase flow appropriate for representing wellhead oil flow?

   b. What are the thermophysical and chemical properties of the crude oil? How are those properties captured, or not captured, by the simpler fluids used in the study?
   c. Wellhead conditions were applied based on results from a worst-case discharge (WCD) model by Hilcorp; however, details of this model are either not adequate or not provided.
2. Naturally imposed external flows were not considered.
3. The verification and validation process was not rigorous.

The committee suggests that a broad-based research program may be appropriate to address the complex challenges of wellhead combustion. To this end, identifying better unit problems to frame such a research program will require more substantive understanding of the underlying conditions of wellhead combustion, as well as the goals for the stakeholders of such work.

1

Introduction

The National Academies of Sciences, Engineering, and Medicine was requested to conduct a peer review of *OSRR 1063: Bureau of Safety and Environmental Enforcement Report: Computational Fluid Dynamics Model for Predicting Wellhead Oil-Burning Efficiency at Bench and Intermediate Scales: Interim Report* (July 30, 2020), produced by the U.S. Naval Research Laboratory (NRL) and funded by the Bureau of Safety and Environmental Enforcement (BSEE). The work was carried out by an ad hoc committee convened by the National Academies and overseen by the Board on Chemical Sciences and Technology within the Division on Earth and Life Studies. The committee's peer review encompassed the study methods, the quality of the data informing the study, and the strength of any inferences drawn by the NRL authors; accordingly, this final peer review report focuses on the technical nature of the interim NRL report (OSRR 1063).

CONTEXT FOR THIS PEER REVIEW

BSEE is responsible for permitting, oversight, and enforcement of the laws and regulations governing offshore oil and gas development. Within BSEE, the Oil Spill Preparedness Division (OSPD) is responsible for developing and administering regulations related specifically to the oil and gas industry's preparedness to contain, recover, and remove oil discharges from facilities operating seaward of the coastline. As part of its permitting authority, BSEE must certify that operators are prepared to respond in the event of a loss of well control and a "worst-case" release.

OSPD is in the process of reviewing a proposal by an independent operator to use wellhead burning to mitigate the effects of a potential well blowout from a gravel island in federal waters off of the North Slope region of Alaska. Because BSEE is charged with ensuring that offshore oil and gas development occurs with minimal environmental impact, it is critical that permitting, oversight, and regulatory decisions be based on the best available science. Therefore, as part of the review process for the independent operator's proposal, BSEE contracted with NRL to conduct a literature review and provide preliminary technical guidance on the feasibility of wellhead burning as a mitigation method. This review demonstrated insufficient evidence in the published literature to support the proposal that wellhead burning would be efficient enough to minimize unburned oil fallout. BSEE subsequently contracted with NRL to conduct a research program with the primary objective of developing a computational fluid dynamics (CFD) model, with experimental validation at multiple scales (bench scale to intermediate scale), of the burning efficiency of wellhead flames. BSEE asked the National Academies to conduct an independent peer review of NRL's interim report on the CFD model and experimental validation results.

THE COMMITTEE, ITS TASK, AND ITS APPROACH

The peer review of *OSRR 1063: Bureau of Safety and Environmental Enforcement Report: Computational Fluid Dynamics Model for Predicting Wellhead Oil-Burning Efficiency at Bench and Intermediate Scales: Interim Report* was conducted by a carefully selected committee of experts appointed by the President of the National Academy of Sciences. The committee included experts in wellhead condition assumptions; flow, soot, and radiation models; droplet injection models, imaging techniques, and characterization; laboratory test validation; temperature measurements; flow regime impact on effluent plume; wellbore flow impact on plume; fire plume and flame projections; and burn efficiency. See Appendix E for biographical information on the committee members.

To carry out its statement of task (Box 1-1), the committee reviewed NRL's interim final report, as well as additional background information provided by BSEE, including a detailed list of charge questions for the committee to address (see Appendix A). To conduct a thorough peer review, the committee considered salient information in the published literature. The committee's deliberations were confidential to avoid any political, special-interest, or sponsor influence. Checks and balances were applied throughout the process to protect the integrity of this report.

BOX 1-1 Statement of Task

The National Academies of Sciences, Engineering, and Medicine will convene an ad hoc committee to review *OSRR 1063: Bureau of Safety and Environmental Enforcement Report: Computational Fluid Dynamics Model for Predicting Wellhead Oil-Burning Efficiency at Bench and Intermediate Scales: Interim Report* (July 30, 2020) produced by the U.S. Naval Research Laboratory (NRL) and funded by the Bureau of Safety and Environmental Enforcement (BSEE). Specifically, the committee will comment on:

- The technical quality and completeness of the interim final report;
- The assumptions and approach used to develop the computational fluid dynamics (CFD) model; and
- The completeness of the modeling results and experimental validation as an evidence base for determining whether wellhead burning is sufficient for mitigation of uncontrolled environmental release of oil in the event of loss of well control.

To accomplish its task, the committee held four virtual meetings, including two data-gathering sessions that included presentations by NRL and BSEE staff. Both data-gathering sessions were open for the public to access; agendas for those sessions are provided in Appendix C.

Shortly after its official appointment, the committee was provided with the NRL interim report, supplementary materials, and the charge questions supplied by BSEE. Each member was asked to answer the charge questions based upon their findings and interpretation of the interim report. These answers were submitted to staff for compilation and distribution to the full committee prior to its final meeting, when the members reached consensus on a response to each question.

ORGANIZATION OF THE REPORT

Chapter 2 presents the committee's consensus answers to BSEE's charge questions. The committee members' individual anonymized answers to the questions can be found in Appendix B. The committee's findings and conclusions are presented in Chapter 3. The charge questions were used to guide the committee's thinking about its Statement of Task, and the committee did not limit its discussions to those questions. After considering the answers to the charge questions, the committee determined what additional information was needed to address each bullet of the Statement of Task.

2

The Committee's Responses to the Charge Questions

This chapter represents the committee's consensus answers to targeted charge questions provided by the Bureau of Safety and Environmental Enforcement (BSEE) as a frame for the committee's assessment of the interim report prepared by the Naval Research Laboratory (NRL). Chapter 3 expands on broader comments on the interim report addressing the committee's statement of task (Box 1-1 in Chapter 1).

Were the objectives of the study clearly defined?

The description of the objectives in the NRL interim report lacks detail and fails to provide a broader context regarding the relevance of the study to the problem at hand. These contextual gaps include laboratory-scale and computational fluid dynamics (CFD) validation, especially with respect to scaling up to relevant physical scales in which buoyancy and radiation depend on the physical dimensions of the wellhead. There is no explicit characterization of the relevant nondimensional numbers of the real-world problem when the bench- and intermediate-scale experiments are compared. In particular, radiation will be increasingly important at larger scales, whereas conduction and convection may dominate at the bench scale.

Relatedly, explanations for why the set of fuels was selected for study are limited, and the relevance of these fuels to the expected multicomponent crude oil is unclear. Important processes—e.g., vaporization properties, surface tension, and preferential evaporation missing in a single-component spray—may have been overlooked by this selection. This work appears to have placed emphasis on the lighter end of the spectrum of hydrocarbon components found in crude oils, whereas if what falls to the ground is the priority, the fuels considered need to include heavier hydrocarbons.

One important clarification in the modeling objectives is whether the selection of submodels is intended for engineering calculations or for high-fidelity models that would be used for more scientific analyses. Some of the assumptions provided for the submodels are significant and not necessarily state of the art.

It would also be useful to clarify the manner in which the efficacy of the different submodels would be determined. This clarification would be bolstered by a discussion of whether the choice of submodel is likely to under- or overestimate the burn efficiency, as well as of the sensitivity of burning efficiency to the submodels and tunable parameters within the submodels.

Were the assumptions regarding wellhead conditions and two-phase wellbore flow (including film thickness and instability, liquid entrainment, and droplet diameter and its influence on wellhead ejection behavior) adequately characterized?

Earlier sections of the report include a good discussion of wellhead-spray combustion scenarios. However, the authors do not clearly justify their choices of the submodels and the values of their assumptions, nor do they cite adequate references. Few assumptions on the selection of properties are specified. In the absence of detailed correlations for property estimation, the assumptions may be fine, but the modeling and experimental work do not validate the properties used. The two-phase wellbore flow modeling was focused on film thickness, entrainment, and droplet diameter, but the role of these parameters in combustion efficiency was not established, and it is unclear that these parameters are sufficient to describe combustion efficiency (quantitatively or qualitatively).

The authors assume annular-mist flow behavior for the sake of brevity and applicability, as these sprays may atomize well. However, the pools or fountains emerging from lower speed flows may not burn well, as evidenced by the authors' experimental results. Thus, the modeling they performed may not have considered the "worst-case" conditions for combustion efficiency (i.e., conditions in which significant oil droplets drop out of the flow).

Knowledge of the range of nondimensional parameters expected in multiphase wellbore flow and a review of the literature on the regimes of the transition flow in wellbores would help clarify how relevant the authors' assumptions are for the wellbore flow. The authors provide a reasonable review of the literature on correlations for film thickness, liquid entrainment, and droplet diameters. However, it is not clear whether those correlations are valid for the regimes under consideration. Additionally, while the correlations for Weber numbers may be valid for the bench-scale simulations, it is unclear whether they are applicable for the actual wellhead.

A fundamental and critical concern is the model used to generate the input conditions for the NRL model. The worst-case discharge (WCD) model from Hilcorp is proprietary (per the Hilcorp report, whose Appendix G is not provided). Thus, detailed data, such as the content listed in the Society of Petroleum Engineers Technical Report,[1] including flow correlations and uncertainty ranges of the parameters used in the Hilcorp WCD model, are not provided for evaluation. The choice of modeling methods will affect outputs from the Hilcorp WCD model, which were used as input conditions for the NRL model. Perhaps it is possible for BSEE to provide input ranges used for the WCD model for the particular reservoir of interest in the NRL study so there is some control on the input, initial, and boundary conditions used with the NRL model. Moreover, the WCD model emphasizes volume flow rate and does not consider dimension predictions for annular-domain inner radius, spray/mist character in the central core of the pipe flow, or the liquid structures that form in the pipe-exiting cascade process. These aspects will affect atomization or liquid-stream breakup.

Alternatively, the Hilcorp report includes some information on reservoir rock and fluid properties (Section 4) and well design (Section 8), among other data that could be used to build an independent WCD model. An independent model would require additional analog and dynamic data, but would be useful to verify output from the Hilcorp model and to cross-validate the WCD output of different wellbore flow models. Such verification and validation would help characterize the wellhead conditions and provide uncertainty bounds for the NRL study.

A related critical concern is the conditions during actual drilling. During actual drilling, if reservoir or flow conditions changed, the WCD model and the associated results would need to be updated. The uncertainty associated with such a scenario would affect outflow and wellhead conditions, leading in turn to questions about whether wellhead burning will suffice as a response plan in all unpredicted situations.

Key expertise on WCD model building and wellbore hydraulics appears to have been lacking in the NRL study. Important research reports on WCD could help guide and inform future modeling and experimental work on this subject (see Appendix D).

Lastly, the NRL interim report does not address the roles of actual wellhead failure geometry and interference of the flow discharge with superstructure. The condition and type of exit structure can affect the external flow, so the systems used in the modeling and experimental work require justification.

Was the physical model for multiphase flow adequately developed to capture the liquid droplet phase and the gas-phase flow field?

It is unclear whether the collective physical and computational aspects of the NRL modeling are appropriate for predicting the actual wellhead conditions in the field, as opposed to predicting the bench- and intermediate-scale experiments that were conducted. The bench-scale problems could be considered as an initial set of unit problems representing the wellhead conditions and opportunities to investigate the

---

[1] Society of Petroleum Engineers. 2015. *"Calculation of Worst-Case Discharge (WCD)."* SPE Technical Report Rev. 1.

significance of parameters relevant to each unit-scale enquiry. Even the bench-scale problem has significant complexities, and while the authors are reasonable in their preliminary approach, a number of issues remain as relates to the relevance of the selection of models and their validation in terms of the subprocess models, uncertainty quantification, and sensitivity analyses relative to the parameters given. The selection of the CFD models using conventional Reynolds-averaged Navier-Stokes (RANS) approaches and subprocess models is justified based on computational costs and time constraints. Nonetheless, the subprocess models were taken off the shelf with little further development, and the NRL interim report contains sufficient information to show that further development is needed based on the droplet dynamics and combustion data. Given the complexity of the overall problem, subprocess models must work in tandem, and it would have been preferable to provide sensitivity and uncertainty quantification of model assumptions, constants, and boundary and initial conditions as they relate to the ultimate objective of predicting burn efficiency. The report would benefit from a more extensive review of the literature on flow, physical, and chemical properties observed under wellhead conditions to guide the selection of further experiments and CFD models.

Were the soot and radiation models adequately characterized?

The sooting and liquid-phase coke particulate emission characteristics of crude oils are not well represented by n-heptane. Particulate generation and burnout will affect several critical physical and chemical transport mechanisms in the model, including the radiative energy balance. In addition, preferential evaporation of lighter components in crude oil may induce composition and thermal stratification in the mixture not captured by n-heptane, which affect combustion rates. CFD mixing and combustion models need to account for this stratification. While use of a surrogate may be a necessary approach for representing crude oils, the committee had considerable concern regarding how to appropriately develop and validate surrogates for studies of crude oil combustion. Developing a surrogate that could be reproduced by other members of the community for complementary studies would be valuable. Such a surrogate would need to reproduce the relevant properties of crude oil, including viscosities, surface tension, latent heat, boiling point, and heat of combustion. Existing crude oil distillation and chemical properties show the extent to which internal liquid cracking and gasification must vary (as a result of changes in distillation fractions with temperatures exceeding 350 ºC) for oils located just tens of miles distant from one another. Much greater effort to characterize and understand the physicochemical property effects of crude oils on atomization and combustion will be needed if the proposed model is to be used for regulatory applications, as proposed by the sponsors. This work would likely require better understanding of current oil property tests and the development of new standardized tests (e.g., by ASTM) specifically suited to crude oils.

In addition to an oil surrogate, the study would be greatly improved by the inclusion of a laminar configuration for parametric studies. The laminar flame configuration would benefit from two types of studies: volatilized combustion and spray flame combustion of the surrogate under different conditions that could test effects of entrainment of cold air. Further suggestions include studying effects of turbulent cross-flow at typical Arctic wind speeds, and potentially leveraging data from large-scale pool fires with wind in the literature and perhaps available from other National Laboratories. However, understanding the cross-flow and discharge ratios of these experiments compared with the NRL system is critical to their utility in model development.

Some specific suggestions for improving the soot and radiation submodel characterization include using a blend of sooting propensity materials (including aromatics and aliphatics) without coking potential to develop a simple soot model that could be validated. The soot submodel needs to be validated using laminar flame configuration and by comparison with the sooting flame data in jet flames from the International Sooting Flame Workshop.[2] The submodel could be validated using any of a number of soot

---

[2] International Sooting Flame Workshop. n.d. *Data Sets*. The University of Adelaide. https://www.adelaide.edu.au/cet/isfworkshop/data-sets.

measurements, such as luminosity, extinction, or laser-induced incandescence.[3] Another potential approach to validating the soot submodel is searching the literature for information on smoke point for similar fuels and reproducing the data for the surrogate (see Appendix D for suggested resources).

Assessing soot production and radiation with entrainment of air of different temperatures is an example of how to provide valuable information on the sensitivity of the submodels to such input parameters as the colder air temperatures expected in the Arctic. Sensitivity analysis is critical to understanding the effects of model input uncertainties.

Were Lagrangian droplet dynamics and thermophysics adequately incorporated into the model?

Use of a combined Eulerian-Lagrangian approach appears to be the appropriate choice for modeling the droplet dynamics. However, significant physical contributors were missing from the modeling effort. For example, while there was some attempt to validate this aspect of the model, it was not based on droplet dynamics. In fact, the droplet trajectory and velocity were not measured, although it may be possible to analyze the data collected in the experiments to determine this information quantitatively. Additionally, the dynamic model was inadequate; it did not account for gravity/buoyancy, assuming that Stokes drag for large droplets in air is incorrect, and proximity to other droplets was not accounted for. Also not accounted for were other thermophysical phenomena, such as internal droplet heating and circulation, as well as preferential evaporation and swelling, which may induce stratification that affects combustion rates. Some of these phenomena may not be important; however, characteristic length and time scales are necessary to justify omitting or including them in the model and submodels. Fundamentally, the model and submodels are semi-empirical and were not developed or tested for oil well fires, nor were sensitivity and uncertainty due to model assumptions and input parameters analyzed; therefore, high uncertainties are likely.

Other concerns about modeling of the droplet dynamics include the initial conditions and the fuel choice. It would have been useful as well to model the flow in the pipe and use it as initial conditions. Pipe exit geometry effects may also affect the exit flow (e.g., spray characteristics, flow rate). Experiments could explore such features as jagged protrusions and inward or outward tuliping of the pipe to understand how important these issues are. Additionally, representing crude oil using a single-component heptane is unsuitable because the heptane is too light and has specific associated sooting propensity due to its chemical structure; hence the sooting potential and characteristics will be different from those of crude oil.

Does the droplet injection model adequately simulate realistic diameters and velocities of two-phase, high-speed flows that would occur during a wellhead blowout event?

In the absence of data for the two-phase flow in the pipe and injection plane, the authors made a series of clearly stated assumptions. The experiments and simulations were performed at scales that differ significantly from those in actual oil well conditions. Attempting to account for scale effects by performing experiments at different scales is the proper approach. However, it is unclear and hardly discussed whether the laboratory droplet diameters and velocities (which were not measured) are relevant to actual wellhead conditions, which are extremely difficult to achieve. Differences in scales and breakup regimes, including thermal effects, are likely to generate very different droplet statistics and dynamics. Other potential significant effects include primary and secondary breakup, and deformations. The choice (or validation) of the model constants was not evaluated and is not discussed in the interim report. Cross-flow winds could also play a significant role in the droplets' breakup and transport, and some evidence exists in the literature about how breakup mechanisms change as Reynolds number and Weber number change. The values of these parameters in the domains for the two scales of experiments and in the third domain related to the practical field need to be compared.

---

[3] Michelsen, H. A. 2017. Probing soot formation, chemical and physical evolution, and oxidation: A review of in situ diagnostic techniques and needs." *Proceedings of the Combustion Institute* 36(1):717-735. DOI: https://doi.org/10.1016/j.proci.2016.08.027.

Does the validation process capture the controlling physical properties to a sufficient level of accuracy including transport and boundary conditions at the bench- and intermediate-scales for both gas-phase and two-phase turbulent spray?

There was general consensus among the committee that the validation process did not capture the controlling physical properties; however, the committee also recognized that validation of such complex fuels, processes, and models is challenging. While the experimental progression is well described in the interim report, discussion of quantitative validation is limited. The experiments provided some valuable information; however, they did not target validation of specific submodels.

Radiation and soot formation submodels were not appropriately validated, and these phenomena are expected to have significant effects on combustion efficiency and dimensionality, among other plume characteristics. In particular, heptane is not a high-sooting fuel, and its sooting propensity is not expected to be consistent with that of wellhead fuels. Other fuels, such as a higher-sooting-propensity single-component fuel (e.g., toluene) or mixtures of such a higher-sooting fuel with heptane, could be used to assess experimentally the effects of sooting propensity on the plume characteristics and observable features. (See the suggestion to create a soot surrogate fuel under the above discussion of soot and radiation models.)

The experimental studies were not specifically directed at validation for specific submodels. Like the radiation submodel, the turbulence combustion closure submodel lacks justification and validation, and there are similar concerns regarding the droplet model. A fundamental concern is the primary assumption about using two-dimensional axisymmetric modeling for what is a highly three-dimensional physical flow. This assumption also has not been validated; horizontal wind speeds in the Arctic are very high, and cross-flow is expected to make wellhead flames highly nonaxisymmetric. The large-scale motion of the macroscopic flows and how they are coupled with the smaller-scale fluid motion have not been validated and may be a significant omission from the modeling and experimental validation efforts. The effects of turbulent mixing and the associated closure models (e.g., progress-variable scalar dissipation rate, mixture fraction dissipation rate, and cross-dissipation rates) also were not modeled and are not discussed in the interim report. Given the significant stratification expected with wellhead flames, these effects will very likely be important in determining the predicted combustion efficiency.

Other concerns relate to (1) transient heating and vaporization of the droplets, including the effect of shear-driven internal circulation within the droplet; (2) multicomponent mass diffusion within the liquid; (3) the importance of group droplet behavior in contrast to the assumption of isolated-droplet heating and vaporization; and (4) the mode of liquid-stream breakup (e.g., lobe-ligament-droplet cascade, lobe-hole-bridge-ligament-droplet cascade, or some other sequence). Understanding the size of the droplets expected would help in assessing the importance of these transport mechanisms.

Were the phase Doppler anemometry imaging diagnostic methods for the droplet behavior measurements appropriately designed, clearly described, and adequate to capture droplet behavior for the Gas Phase and Two-Phase Spray Flame?

There was agreement on phase Doppler anemometry (PDA) being appropriate, with some caveats with respect to the range of its use. The PDA system and the measurement technique are described well in the interim report. The results are valuable for providing insight into the structure of the flow. The PDA system results are not useful near the exit plane because the liquid still has a sheet or ligament-like structure; they are useful only when the spray is composed predominantly of spherical droplets. Additionally, the data plots lack error bars. Regarding the interpretation of the data, on page 61 of the interim report, the authors state that there were essentially no droplets outside r = +/–4 mm; however there were enough droplets to obtain a velocity reading, which appears to represent an inconsistency.

Were the diffuse back-light illumination imaging diagnostic methods for the droplet behavior measurements appropriately designed, clearly described, and adequate to capture droplet behavior for the Gas Phase and Two-Phase Spray Flame?

The diffuse back-light illumination imaging was appropriately designed and provided meaningful insight and some data on the shape of the droplets and plume configuration, elucidating some of the initial breakup processes. The procedures are described adequately in the interim report. However, the report does not use the data for characterizing the droplet dynamics, other than showing one sample demonstrating a capability to track the droplets. Much more information—e.g., droplet velocity and size distribution—could be obtained by dynamically postprocessing the data. The interim report provides only preliminary results, with detailed analysis left for future investigations. An uncertainty analysis and assessment of accuracy are also absent.

Were the diagnostic methods (Coherent Anti-Stokes Raman Spectrometry-based Thermometry [CARS]) for the temperature measurements appropriately designed, clearly described, and adequate to capture temperature for the Gas Phase and Two-Phase Spray Flame?

The committee reached general agreement that the Coherent Anti-Stokes Raman Spectrometry-based Thermometry (CARS) method was competently applied and appropriate for the experiments and is well described in the interim report, with the caveat of suggesting improvements to the analyses. Specifically, the authors need to do a more thorough uncertainty analysis for their CARS measurements. This is a much more complex task than that for the previously discussed PDA measurement. Figure 45 in the NRL interim report appears to indicate that uncertainty analysis was done for data from the particular flame that was investigated, with 0.1 g/sec of ethane and 0.2 g/sec of heptane. The authors need to explain how they determined these uncertainties and include uncertainty bars on Figures 28 and 30 as well. They also need to explain clearly the differences between the averaged and single-shot measurements shown in Figure 53. For future CARS measurements in this group, it is essential to further develop the computational framework for analysis of single-shot CARS spectra.

Were the diagnostic methods (3-Color High-Speed Pyrometry) for the temperature measurements appropriately designed, clearly described, and adequate to capture temperature for the Gas Phase and Two-Phase Spray Flame?

The assessment of this technique and the results needs to incorporate uncertainties in the measurements, particularly in comparison with CARS gas-phase measurements. The 3CHIP method for temperature analysis of soot raises some issues, as does the interpretation of the results. First, the emissivity of soot changes dramatically with maturity. Lower in the flame, where the soot is less mature, the dispersion exponent ξ will be much larger than 1; that is, the emissivity is proportional to $1/\lambda^{\xi}$, where $\xi >> 1$ for young soot. Using a value of ξ that is too small will lead to overprediction of the temperature. Soot will age and mature with increasing height in the flame. In normal diffusion flames, soot is also often more mature at the flame front at higher radial distances. At full maturity, the dispersion exponent is less than 1 ($\xi < 1$), and using the value of unity will lead to underprediction of temperature. Thus, the trend for temperature may be the opposite of that suggested in Figure 30 of the interim report for the particulates as a function of height in the flame, considering the change in optical properties with soot maturity. Along the edges of the flame, optical dispersion effects may highly perturb the 3CHIP measurements because of the refractive index changes with temperature. Finally, it is highly unlikely that soot will have a different temperature from that of the gas phase at atmospheric pressure because conductive heat transfer equilibrates temperatures on timescales of nanoseconds at such pressures. In addition, if there are interactions between less volatile crude oil and soot particles, optical properties of the internally mixed particles will deviate from those of mature soot and look more similar to those of young soot, leading to larger deviations from a $1/\lambda$ dependence of the emissivity and significant errors in inferred temperatures. Furthermore, for high-sooting conditions, luminosity measurements need to be corrected for reabsorption.

Do the results adequately characterize evidence of the droplet characteristics including droplet breakup, the droplet size (diameter), droplet speed, and the duration of droplet in fire (bench- and intermediate-scales)?

There are significant disconnects between the model and the attempts to validate it. The work does not demonstrate key aspects of the models such as interactions between droplets, roles of convection, and radiation or gravity effects (including natural convection and falling droplets). The relevance to wellhead fuel properties, flow conditions (annular vs. bubbly, emulsions) is missing. The authors provide high-quality images that could prove insightful quantitative and qualitative information on the droplet breakup and modeling assumptions, but did not analyze those images showing droplet fragmentation, including interpretation of the behavior of the droplet breakup, the droplet velocity, or a characterization of the relevant physical conditions. Further analysis of the imaging data is needed, as recognized by the authors.

Does the research product accurately expand predictions of droplet diameters beyond current limited validated ranges?

In the introduction to the interim report, the authors acknowledge the importance of scaling and discuss relevant dimensionless parameters, but they did not appropriately address this issue with analysis and experimental results, nor did they attempt to extrapolate the results between their two experimental scales or to full-scale conditions. A wealth of data from experiments performed by the authors could have been used to address scaling trends, but the authors did not perform this work, and did not use the experimental data well to examine the key assumptions about isolated droplet vaporization and heating and the effect of shear force on droplets. Are droplets batched together sufficiently to require the use of group theory for vaporization and burning? If nonspherical droplet shapes appear, shear could be one cause, thereby also being a likely cause of internal droplet circulation that would strongly affect heating and vaporization rates.

Does the research product accurately characterize the impact of two-phase flow regimes (bubble, slug, and churn) on the effluent plume (bench- and intermediate-scales)?

A clear outline of the two-phase flow characterization is critical because it directly impacts burn efficiency, defined as the amount of liquid that falls to the ground. While the experiments were configured around annular flow of liquid coming out of a pipe with some spray in the center, the interim report does not clearly present the evidence for the assumption of this regime. This assumption is critical to the manner in which breakup occurs, so it is difficult to discuss impacts of the flow regime on atomization unless one knows whether there is annular or bubbly flow.

Justification for the assumption of annular flow is necessary, whether experimental limitations or expectations of output from the wellhead. This assumption would have been strengthened by a more robust literature review on two-phase flows through wellbores. Another concern is whether there may be a water phase, which, in addition to making this a three-phase flow (water, oil, gas), would allow for the possible formation of oil-in-water and water-in-oil emulsions. Addressing how this would impact the modeling results would strengthen the model's applicability to other reservoirs as well, even if water intrusion is not a concern here. See Appendix D for literature on this topic.

More explicitly, in this instance, because the Hilcorp WCD model is proprietary, no details are provided. Information on pipe flow and wellbore model details and types are also missing, as is the application of key expertise in wellbore pipe flow and WCD modeling and experimental research. There is no way to verify whether the WCD volume is valid. Hence, a great deal of uncertainty is associated with the WCD model used for input to the NRL model, and it is unclear how the authors dealt with this uncertainty. This is not a small matter; indeed, it likely controls or limits the model predictions. Even if Hilcorp is unwilling or unable to provide specifics, identifying a range of values with confidences with the help of oil experts would enable NRL to build its own WCD model. Valuable references relevant to wellhead modeling, particularly Waltrich et al. (2019) and Society of Petroleum Engineers (2015), are included in Appendix D.

Does the research product adequately address how the wellbore flow would influence the ejected spray plume behavior, which directly influences how the oil and gas burns and how much will either fall back to the surface or remain vapor?

The committee reached agreement that this research product does not adequately address how the wellbore flow would influence the behavior of the ejected spray plume. The initial experiments are foundational, but need to be expanded based on the current limited observations and limited conditions considered. Furthermore, the envelope of conditions needs to include the range of physical properties expected for crude oils, including highly volatile dissolution and water in the fluid. Such experimental pursuits are important to enable ranking and prioritizing of the physical mechanisms that should be included in the model development and consideration of property ranges.

The committee has significant concern that the variability of oil composition dramatically affects many aspects of wellbore fires, including the pipe flow. If the goal is to create a model for a broad range of crude oils, the effects of the different thermophysical properties (e.g., surface tension, volatility, heat capacity) need to be considered. If the goal is to create a model for a more specific type of oil, then the range of oil properties needs to be summarized, and the experiments need to reflect that range of properties. Pipe geometry can likely play a role as well (e.g., shear flow, boundary layer effects). What are the geometric features of the wellbore exit (tapered pipe, flow bends)? Identifying the key pipe attributes required for the boundary conditions is a critical first step in designing the modeling approach and the experimental efforts. Additionally, detailed simulations of different pipe flow conditions are important to improve understanding of the behavior of the ejected spray plume. Emulsified materials may also be a relevant consideration (e.g., what water content is expected in the oil flows?).

While these are significant concerns, the experimental setup could potentially be used to study these effects, such as the role of pipe boundary layers and different crude oils, information that could be used to help understand the magnitude of the effects. Similar to the experiments, the subprocess models (turbulence, combustion, radiation, soot, spray) need to be individually validated against unit test experiments with well-characterized inlet boundary conditions for the envelope of relevant conditions before the combined effects are tested.

Does the research product accurately predict the length of fire plume, location of flame anchoring, height of flame, width/angle, expansion, etc.?

Evaluation of the fire plume dynamics is complex and heavily dependent on the submodels used and developed for liquid- and gas-phase transports. The authors incorporated some of these issues of elemental physics, albeit in the form of model parameters. However, they made many assumptions for the study. In particular, the width/angle of the liquid sheet was used as an input instead of being evaluated with a physical model, which leads to restriction in such parameters as flame dynamics, flame stability, and lift-off height. For flame calculations, tabulated values were used. This method requires that the fuel composition be known as droplet evaporation proceeds, thus necessitating a more detailed multicomponent droplet evaporation model. The authors implemented a simplified droplet evaporation model, which could lead to uncertainties in flame height. Furthermore, the real wellhead conditions with heavy fuels may not be realized with these simplified assumptions.

The authors provide only trends for such parameters as location of flame anchoring and height of the flame, and no detailed results from simulation and experiments, or their comparisons. Additionally, they conducted their investigations within a narrow range of flow conditions, so it is unclear whether the results can be related directly to the high-flow-rate condition of the wellhead, where blow-off may occur. Limiting conditions for ignition need further exploration as well.

The authors developed a reasonably robust code that could be used in the future to investigate various parameters. More accurate submodels could also be included in future work.

Does the research product determine the primary mechanism driving burn efficiency?

The authors investigated the breakup dynamics of the liquid phase and the gas-phase combustion of atomized droplets to obtain the "burn efficiency." Results of the intermediate-scale experiments show that the large droplets fall back to the ground because of their weight. In the modeling approach, some of the underlying physical processes were captured, albeit with empirical correlations. But the experiments did not address the extent to which the droplet size distribution might be skewed by pipe exit geometry and fracture protrusions. The structure of the exit may need greater consideration given that the dropout of large drops appears to be significant.

The flamelet model with a progress variable is a widely used model, but has large uncertainties caused by significant assumptions that are likely wrong. The model relies only on normal rate of strain in the flow and neglects any effect of shear strain and vorticity. At the same time, there is no direct and clear relationship between strain in the Large Eddy Simulation (LES) field and scalar dissipation in the flame; only a vague connection is made in flamelet theory. Unfortunately, a better model is not quite yet available. Still, the NRL report needs to identify the inherent weaknesses of the flamelet model.

The axisymmetric nature of the model may also pose some limitations. Depending on the exit conditions at the wellhead, nonaxisymmetric gas-phase plume structure may evolve in realistic wellhead fire scenarios. Axisymmetric models such as that presented in the NRL report cannot capture the burning efficiencies of such cases. The ambient wind conditions and directions can significantly affect the axisymmetric assumption.

Gas-phase models may not be adequate with inherent evaporation/atomization assumptions. Droplet size distribution is input to the gas-phase combustion model and is a questionable choice. The postulated worst-case scenario, which assumes a slower gas velocity, leads to lower liquid atomization and lower burn efficiency. However, higher gas velocities could lead to more entrainment, and gas-phase combustion could become the controlling mechanism.

The authors concluded that the remnant fuels on the ground are primarily from large liquid fragments, which were not entrained into the flame and settled because of heavier weight. However, the choice of surrogate fuel significantly affects this observation. The mismatch between the distillation range and particulate mass generation potential (and radiation effects) between the simpler surrogate fuels used for the NRL study and the actual crude properties will likely influence the predicted burn efficiency. Particulate mass generation should include all relevant crude oil combustion particles (e.g., liquid-phase coking, ash, sand, rock). The crude oil is expected to have higher particulate mass generation propensity. Large-scale coke particles will also contribute to the solid/liquid accumulation on the ground.

Sensitivity analysis of the submodels is critical to ascertain the controlling physics that determines the burn efficiency. The NRL report does not provide the needed parametric studies from the computational simulations or the experiments. The current model could be used to perform parametric analysis and determine the sensitivities of various physical processes that control the overall burn efficiency. Furthermore, such analysis in conjunction with experiments could be used to develop a more realistic "burn efficiency" definition that could be used in practical situations.

Were the conclusions based on the OSRR 1063 study findings in the report logical and appropriate based on the results?

This is a very difficult research problem, and the authors performed foundational work for modeling and experimental research on some of the physicochemical mechanisms for physically downscaled wellbore processes. They identified some of the important aspects to be considered and developed some foundational understanding of physical and chemical processes relevant to wellbore ignition and combustion problems. Details and scaling remain to be done, so the applicability of this work to full scale is still unclear.

At the core, there are concerns about the omission of certain information in the model—e.g., buoyancy, droplet size and velocity distributions, spray falling to the ground, and the potential for a fire whirl—that would have been relevant to the resulting burn efficiency. Additionally, even in the CFD model, a great deal of uncertainty in the submodels was not characterized. Submodel assumptions were not validated, and grid convergence and numerical artifacts also were not well characterized with respect to the submodels. It is therefore difficult to determine whether discrepancies exist and if so, whether they are attributable to numerics and resolution versus inadequacies in the model. In addition to validating the submodels, performing a sensitivity analysis would elucidate the impact of the different submodels on the end result. At this stage, this model is not predictive.

The bench-scale experiments the authors performed were largely experimentally correct, with competently executed measurements (although there were issues with the 3CHIP measurements). However, the authors conducted no diagnostics other than imaging for intermediate scale. The results also do not link clearly to larger scales, from lab scale to meso/room size. Extrapolating these results to the wellhead is problematic, in no small part because of differences in the behavior of the model oil chosen and crude oil. The work would have benefited from a range of nondimensional parameters and some idea about effects of different physical and chemical properties of n-heptane relative to the range of crude oil properties expected in the field.

Overall, the results and comparisons between the experiments and computations are limited, and their relevance to real-world wellhead oil burning is questionable. Many of the conclusions are observational and not in dispute. Conclusions assessing whether this technique will work in the field are lacking. This body of work does not provide a concrete foundation for determining whether wellhead burning is sufficient for mitigation of uncontrolled environmental release of oil in the event of loss of well control.

3

Conclusions

The goal of this project to predict the combustion efficiency of wellhead flames was ambitious, and the Naval Research Laboratory (NRL) report shows that both modeling and experimental frameworks have been successfully initiated and are ongoing. Without a well-defined problem, however, it is difficult to define all of the submodeling components and their required complexity so as to meet the goals expressed by the sponsors of the work. Furthermore, it will be difficult to improve the modeling and experimental programs without more concise information and consideration of the variability of the physical and chemical properties of crude oil that appear to be of interest in terms of future predictive uncertainties and the foreseen utility of the NRL model.

The committee identified key concerns regarding the NRL modeling approach and experimental methods in three categories:

1. Gaps in the study approach and the assumptions chosen to represent the physical system of wellhead combustion limit the utility and accuracy of the approach and the model.
2. Several modeling approaches employed are not the state of the art.
3. Other modeling methods employed are the state of the art, but their related uncertainties and known weaknesses are not considered.

The objective of predicting the combustion efficiency of wellhead fires was not well scoped in the NRL study. The envelope of multiphase flow conditions and the physical and chemical properties of crude oils were not adequately accounted for in terms of submodel property considerations either in developing the model or in choosing fuels to be used in bench-scale experiments. The feedback of results of experimental efforts into the development of submodel component needs, as well as the validation of model predictions, was very limited. Hence, the relevance of the selected laboratory- and bench-scale experiments and computational fluid dynamics (CFD) simulations to actual field conditions remains highly uncertain. While the authors of the NRL report made reasonable a posteriori comparisons between the Reynolds-averaged Navier-Stokes (RANS) CFD and the bench-scale experiment, many of the conventional submodels used and their assumptions were not validated for the conditions at hand, and sensitivities and uncertainties of key quantities of interest to the tunable constants of the submodels and boundary conditions were absent. A more systematic verification and validation approach would have been beneficial and would have instilled trust in the predictive nature and level of uncertainty of the CFD approach to conditions outside of the bench-scale experiment. Future studies would benefit from a community survey (involving, e.g., experts and stakeholders) bounding the relevant conditions of wellhead fires, and from the selection of a set of hierarchical unit problems addressing specific aspects of this complex problem.

Regarding the utility of the approach and assumptions applied in developing the model and its components, the wellhead system is not well defined in the NRL interim report, and the level of accuracy required or desired for the model is never identified. For example, what is considered sufficient for the prediction of combustion efficiency—would an order of magnitude suffice? These are fundamental concerns that dictate which approaches for the modeling and experimental work are acceptable—e.g., whether RANS or Large Eddy Simulation (LES) modeling methods are appropriate or how crude properties are to be considered. Another key concern is the lack of well-defined initial and boundary conditions in the context of wellhead combustion.

Designing appropriate experiments with which to validate the model or help scale the results to actual wellhead combustion conditions is difficult without a well-defined problem. Without a well-defined problem, moreover, it is not possible to evaluate the adequacy of the model.

Other high-level technical findings as to the completeness of the modeling results for predicting wellhead oil-burning efficiency identified by the committee are as follows:

1. It is unclear whether the authors considered the correct flow system.
    a. Are the authors considering the correct configuration for the multiphase flow? Specifically, is co-annular two-phase flow appropriate for representing wellhead oil flow? Can that configuration be justified, e.g., for the range of mass flow, pipe dimensions, fluid properties, and so on? The boundary and initial conditions require justification, and dimensionless parameters (e.g., Re, We) need to be applied to define the system and to leverage work in the literature where appropriate.
        i. The two-phase wellbore flow modeling focused on film thickness, entrainment, and droplet diameter, but the role of these parameters in combustion efficiency was not established, and it is not clear that these parameters are sufficient to describe combustion efficiency (quantitatively or qualitatively).
        ii. The authors provide a reasonable review of the literature on correlations for film thickness, liquid entrainment, and droplet diameters. However, it is unclear whether the correlations are valid for the regimes under consideration. Additionally, while the correlations for Weber numbers may be valid for the bench-scale simulations, it is unclear whether they are applicable for the actual wellhead.
    b. What are the thermophysical and chemical properties of the crude oil? How are those properties captured (or not captured) by the simpler fluids used in the study?
        i. Surrogates may be a good approach for considering certain aspects of the system; however, the current work emphasized lighter hydrocarbon components that will likely significantly affect the combustion efficiency. Specifically, the soot characteristics for crude oil are not encompassed by n-heptane, and sooting propensity will affect several critical physical and chemical transport mechanisms in the model, including the radiative energy balance. In addition, preferential evaporation of lighter components in crude oil may induce composition and thermal stratification in the mixture, affecting combustion rates, which are not captured by heptane, and CFD mixing and combustion models need to account for stratification.
        ii. Few assumptions regarding the selection of properties are specified in the interim report, and the modeling and experimental work did not validate the properties used.
    c. Wellhead conditions were applied based on results from a worst-case discharge (WCD) model by Hilcorp, details of which are either not adequate or not provided. Annular-mist flow regime was considered based on the WCD results and downscaled to apply to the problem at hand. Wellbore modeling methods and input details could be provided to verify output, capture uncertainties, and cross-validate WCD output among different wellbore flow modeling methods, and to improve the assumptions and approach of the modeling and experimental efforts. An independent WCD model could be developed using data from the Liberty (Hilcorp report) and analog reservoirs (for which the Hilcorp report is insufficient). Doing so would help characterize the wellhead conditions and flow parameters and provide confidence in the input/boundary conditions used for the study.
        i. The impact of nonannular flow regimes needs to be considered or justified for exclusion in modeling and experimental efforts.
        ii. Importantly, the authors assume annular-mist flow behavior for the sake of brevity and applicability, as these sprays may atomize well. However, the pools or fountains emerging from lower-speed flows may not burn well, as evidenced by the experimental results. Thus, the modeling may not consider the "worst-case" conditions

for combustion efficiency (i.e., conditions in which significant oil droplets drop out of the flow).

2. Naturally imposed external flows and induced flows were not considered. Specifically, cross-flow was not considered in the modeling or the experiments, and Arctic wind speeds are extremely high (average of 5.5 m/s between September and May on the North Slope, up to 30 m/s during polar lows over the Arctic Ocean, according to the National Oceanic and Atmospheric Administration [NOAA][1]). Buoyancy effects also were not considered, and may be comparable to or exceed the effects of wind cross-flow. These effects may aid or impair burning rates. Additionally, the imposed external flows will lead to significant multidimensional behavior, and the flame/plume evolutions are not well-represented by axisymmetric assumptions. In terms of induced flows, the forced flow of the wellhead fluid at the exit of the pipe will induce external flows that the authors did not consider.
3. The verification and validation processes were not rigorous. For example, the experiments were not designed to validate any of the subprocess models (i.e., the turbulence, turbulence/combustion interactions, combustion chemistry, droplets, radiation, and soot submodels). The sensitivity of the submodels and experiments to boundary and initial conditions was not considered and could provide extremely valuable information to guide future work. There were some opportunities to validate portions of the model with some of the experimental data (e.g., droplet behavior) that were not explored in depth.

The consensus conclusion of the committee is that the model is not adequate for predicting the combustion efficiency of wellhead flames. A broad-based research program may be appropriate to address the complex challenges of wellhead combustion. To this end, identifying better unit problems to frame such a research program will require more substantive understanding of the underlying conditions of wellhead combustion, as well as the goals for the stakeholders of such work.

---

[1] National Snow & Ice Data Center. 2020. *Patterns in Arctic Weather*. https://nsidc.org/cryosphere/arctic-meteorology/weather_climate_patterns.html#:~:text=Wind%20speeds%20average%20around%2050,over%20relatively%20warm%20open%20water.

Appendix A

Peer Review Charge Document

The National Academy of Sciences has been contracted to conduct a peer review of *OSRR 1063: Bureau of Safety and Environmental Enforcement Report: Computational Fluid Dynamics Model for Predicting Wellhead Oil-Burning Efficiency at Bench and Intermediate Scales: Interim Report (July 30, 2020)* produced by the U.S. Naval Research Laboratory (NRL) and funded by the Bureau of Safety and Environmental Enforcement (BSEE). The work will be overseen by the Board on Chemical Sciences and Technology (BCST) in the Division on Earth and Life Studies. The peer review will focus on the methods, data quality, and strengths of any inferences made by the NRL study and as such, the final peer review report will focus on the technical nature of the interim final report (OSRR 1063).

CONTEXT

The Bureau of Safety and Environmental Enforcement (BSEE), within the U.S. Department of the Interior, is responsible for permitting, oversight, and enforcement of the laws and regulations governing offshore oil and gas development. Within BSEE, the Oil Spill Preparedness Division (OSPD) is responsible for developing and administering regulations specifically related to the oil and gas industry's preparedness to contain, recover, and remove oil discharges from facilities operating seaward of the coastline. As part of its permitting authority, BSEE must certify that operators are prepared to respond in the event of a loss of well control and a "worst-case" release.

BSEE's OSPD is currently reviewing a proposal by an independent operator to use wellhead burning to mitigate the effects of a potential well blowout from a gravel island in federal waters off the north slope of Alaska. Because BSEE is charged with ensuring that offshore oil and gas development occurs with minimal environmental impact, it is critical that permitting, oversight, and regulatory decisions are based on the best available science. Therefore, as part of the review process of the independent operator's proposal, BSEE contracted with the U.S. Naval Research Laboratory (NRL) to conduct a literature review and provide preliminary technical guidance on the feasibility of wellhead burning as a mitigation method. Based on the literature review, it was determined that there is not sufficient evidence in the published literature to support the proposal that wellhead burning would be efficient enough to minimize unburned oil fallout. BSEE then contracted with NRL to conduct a full research program, with the primary objective of developing a computational fluid dynamics (CFD) model with experimental validation at multiple scales (bench-scale to intermediate-scale). BSEE is seeking an independent peer review of the interim final NRL report of the CFD and experimental validation results.

As part of its work, NRL developed a repeatable, reliable method to measure burn efficiency. The results of NRL's scientific research are anticipated to be highly influential in the field. Because of this, it is important that the interim final report undergo a thorough, independent peer review to ensure that the methods, data quality, and strengths of any inferences made are based on the best available science.

The primary purpose of this peer review is to assist BSEE in effectively assessing spill mitigation strategies as part of its role in permitting offshore oil and gas development. As such, BSEE will be the primary audience for the peer review report. The peer review report may also be of interest to academic, industry, and government researchers in related fields (e.g., petroleum engineering; chemical engineering; computational fluid dynamics modeling; transport phenomena; combustion science) and private sector companies with interest in Arctic oil and gas development.

Appendix A

PEER REVIEW COMPONENTS

An ad hoc National Academies Committee will provide a peer review of *OSRR 1063: Bureau of Safety and Environmental Enforcement Report: Computational Fluid Dynamics Model for Predicting Wellhead Oil-Burning Efficiency at Bench and Intermediate Scales: Interim Report (July 30, 2020)* produced by the U.S. Naval Research Laboratory (NRL) and funded by the Bureau of Safety and Environmental Enforcement (BSEE). Specifically, the committee will write a report that addresses:

- The technical quality and completeness of the interim final report;
- The assumptions and approach used to develop the computational fluid dynamics (CFD) model; and
- The completeness of the modeling results and experimental validation as an evidence base for determining whether wellhead burning is sufficient for mitigation of uncontrolled environmental release of oil in the event of loss of well control.

As part of the peer review, committee members will respond to the following **evaluation criteria**:

1. Were the objectives of the study clearly defined? If not, what are your recommendations for improving the description of this study's objectives?
2. Were the assumptions regarding wellhead conditions and two-phase wellbore flow (including film thickness and instability, liquid entrainment, and droplet diameter and its influence on wellhead ejection behavior) adequately characterized? Were there any apparent strengths, weaknesses, omissions, or errors? Provide an explanation for your answers.
3. Was the physical model for multi-phase flow adequately developed to capture the liquid droplet phase and the gas-phase flow field? Were the soot and radiation models adequately characterized? Were Lagrangian droplet dynamics and thermophysics adequately incorporated into the model? Were there any apparent strengths, weaknesses, omissions, or errors? Provide and explanation for your answers.
4. Does the droplet injection model adequately simulate realistic diameters and velocities of two-phase, high-speed flows that would occur during a wellhead blowout event? Were there any apparent strengths, weaknesses, omissions, or errors? Provide an explanation for your answers.
5. Does the validation process capture the controlling physical properties to a sufficient level of accuracy including transport and boundary conditions at the bench- and intermediate-scales for both gas-phase and two-phase turbulent spray? Were there any apparent strengths, weaknesses, omissions, or errors? Provide an explanation for your answers.
6. Were the phase doppler anemometry and diffuse back-light illumination imaging diagnostic methods (6.1.1 and 6.1.2 below) for the droplet behavior measurements appropriately designed, clearly described, and adequate to capture droplet behavior for the Gas Phase and Two-Phase Spray Flame? Were there any apparent strengths, weaknesses, omissions, or errors? Provide and explanation for your answers.
    6.1.1.1. Phase Doppler Anemometry
    6.1.1.2. Diffuse Back-Illumination Imaging
7. Were the diagnostic methods (7.1.1 and 7.1.2 below) for the temperature measurements appropriately designed, clearly described, and adequate to capture temperature for the Gas Phase and Two-Phase Spray Flame? Were there any apparent strengths, weaknesses, omissions, or errors? Provide an explanation for your answers.
    7.1.1.1. Coherent Anti-Stokes Raman Spectrometry-based Thermometry (CARS)
    7.1.1.2. 3-Color High-Speed Pyrometry
8. Do the results adequately characterize evidence of the droplet characteristics including droplet breakup, the droplet size (diameter), droplet speed, and the duration of droplet in fire (bench- and intermediate-scales)? Does the research product accurately expand predictions of droplet

diameters beyond current limited validated ranges? Were there any apparent strengths, weaknesses, omissions, or errors? Provide an explanation for your answers.

9. Does the research product accurately characterize the impact of two-phase flow regimes (bubble, slug, and churn) on the effluent plume (bench- and intermediate-scales)? Were there any apparent strengths, weaknesses, omissions, or errors? Provide an explanation for your answers.
10. Does the research product adequately address how the wellbore flow would influence the ejected spray plume behavior, which directly influences how the oil and gas burns and how much will either fall back to the surface or remain vapor? Were there any apparent strengths, weaknesses, omissions, or errors? Explain for your answers.
11. Does the research product accurately predict the length of fire plume, location of flame anchoring, height of flame, width/angle, expansion, etc.? Were there any apparent strengths, weaknesses, omissions, or errors? Explain for your answers.
12. Does the research product determine the primary mechanism driving burn efficiency?
13. Were the conclusions based on the OSRR 1063 study findings in the report logical and appropriate based on the results? What other conclusions related to the study were made and are appropriate? Are there any additional study findings or conclusions that could be drawn from the study? Provide an explanation for your answers.

REVIEW PROCESS

All peer review committee members will receive a PDF copy of the NRL report *OSRR 1063: Bureau of Safety and Environmental Enforcement Report: Computational Fluid Dynamics Model for Predicting Wellhead Oil-Burning Efficiency at Bench and Intermediate Scales: Interim Report (July 30, 2020)*. All review comments will be entered via a web-based interface: [https://survey.alchemer.com/s3/6218414/BSEE-Wellhead-Report-Charge-Question]. Comments should be entered no later than April 12, 2021.

Please remember that all review comments remain confidential until the final National Academies review report is published. Review comments, without attribution, will be published as an appendix (See Appendix B of this report) to the review report. All closed session discussions and deliberations will remain confidential even after the review report is published. All draft report materials are confidential work products of the committee. Only when the review report is publically released can you discuss the report contents (but never the deliberations).

All peer reviewers should be aware of "applicable access, objectivity, reproducibility and other quality standards under federal laws governing access and quality. More information is available at:

- DOI Department Manual "305 DM 3"
- DOI Information Quality Standards
  - https://www.doi.gov/ocio/policy-mgmt-support/information-and-records-management/iq
- OMB Bulletin
  - https://www.bsee.gov/sites/bsee.gov/files/bsee-interim-document/oil-spill-response/omb-m-05-03-final-information-quality-bulletin-for-peer-review.pdf
- Executive Order 12866
  - https://www.epa.gov/laws-regulations/summary-executive-order-12866-regulatory-planning-and-review
  - https://www.archives.gov/files/federal-register/executive-orders/pdf/12866.pdf

Appendix B

Anonymized Committee Responses to Charge Questions

1. Were the objectives of the study clearly defined? If not, what are your recommendations for improving the description of this study's objectives?

- Objectives can be more elaborate. Specific objectives can be reported with steps involved.
- The objective statement is relatively short. It does not clearly outline the actual goal. Perhaps the study's objectives and the overall expectation the review committee had, were not perfectly aligned.
- According to the authors of the report, the objective was to describe their initial model development approach for the project, generate an experimental set of data on a laboratory scale that could be a source of target information for comparison against model predictions, and then elaborate on the comparison. Their main points to be conveyed were with regard to reproducing the spray experimental results found for water and n-heptane. The second objective was to demonstrate a method to define overall combustion efficiency based upon experiments with a crude. Only a single crude was examined in this part of the work.
- It is not clear if the objective of the study is to develop an "Engineering" model (CFD-Code), that is tested and validated, and can be used by the industry, or if it is basically a preliminary study that helps to identify the issues involved in modeling wellhead fire scenarios. Perhaps it should be stated explicitly by the sponsoring agency (BSEE), and the authors of the study that it is a preliminary work and it will be improved further in the future. To the authors' credit, they seem to have identified all the physics that one can think of and incorporated them into their code to varying degrees of accuracy, and they also point out where further research is needed.
- The scaling effects for comparison of laboratory results and the practical problem are not clearly discussed. How is the laboratory scale relevant? The confidence level of the computational results should be explained.
- "The objective of this program is to develop and validate computational fluid dynamic models for predicting of wellhead burn efficiency. This requires a detailed understanding of the fundamental gas and liquid fluid mechanics; droplet formation, convection, and evaporation; and the spray combustion behavior of crude oil relevant to wellhead conditions." page 73 of agenda book

2. Were the assumptions regarding wellhead conditions and two-phase wellbore flow (including film thickness and instability, liquid entrainment, and droplet diameter and its influence on wellhead ejection behavior) adequately characterized? Were there any apparent strengths, weaknesses, omissions, or errors? Provide an explanation for your answers.

- There is a very good discussion of wellhead spray combustion scenario at earlier sections. However, the authors of the report did not clearly justify their choices of the submodels, the values of their assumptions or cited adequate references. Some of the description may appear at times simplistic.
- Few assumptions on selection of properties are specified. In the absence of detailed correlations for property estimation, these assumptions are fine. Assumption of flow behavior is in equilibrium and fully developed is made. Also, for lower velocity flows formation of pools or fountains than well-atomized sprays is assumed and annular-mist flow behaviour is planned to be modelled. Modelling

focus is on film thickness, entrainment, and droplet diameter. These should be fine considering the complexity of the problem and validation data.

- The flow within the reservoir is described, but there is no evidence that indeed these flow regimes exist. Authors assume annular-mist flow behavior for the sake of brevity and applicability as these sprays probably atomize well. However, the pools or fountains emerging from lower speed flows may not burn well at all and may be affecting the efficiency of the wellhead oil-burning. Authors have reviewed the literature well and several correlations from literature are being used for film thickness, liquid entrainment, and droplet diameters. It was difficult for the reviewer to know if these correlations are valid for the regimes under consideration. While these correlations for Weber numbers may be valid for the bench scale simulations, it is unclear if they would be applicable for the actual well-head.
- Most of the assumptions are described clearly in the report. However, the reviewer has a concern that, in some cases, clear justifications behind the assumptions are not stated. For example, the choice of heptane as the primary fuel has not been justified in the report. During Q/A session, such justifications were discussed. Perhaps, the authors should add them in the report as well.
- Methods have been demonstrated for the scale of the laboratory experiments conducted on water, n-heptane as fluids. It is likely that this is sufficient in terms of the objectives that were suggested by the authors themselves, which was to be an initiating study rather than a more developed demonstration of results, with an indication of what remains to be progressed to yield a predictive result. A wide range of issues remains to be evaluated in this reviewer's opinion and there is no discussion of follow on work and its relevance to proofing methodologies. The scale extrapolation of results remains to tested, and the effects of oil/gas/water fraction of the discharge for even steady-state conditions remain to be evaluated.
- The worst-case discharge (WCD) model from Hilcorp is proprietary (per Hilcorp report, Appendix G not provided). Thus, it is difficult to know details of all data (https://spe.widen.net/s/2vjhlrwgrj/spe-174705-tr) , flow correlations and uncertainty ranges of the parameters used in the Hilcorp WCD model. The choice of modeling methods will affect output from these models which are input into the study at hand. That being said, the Hilcorp report includes some reservoir rock and fluid properties (section 4), and well design (section 8) amongst other data that can be used along with analog data and dynamic data as available, to build an independent WCD model to verify output or to cross-validate WCD output amongst different wellbore flow modeling methods to help characterize the wellhead conditions, and determine best method to do so given the problem at hand. At the very least impact of different wellbore models or flow regimes can be included.
- The theory is based on the behavior of an isolated isothermal droplet without consideration of transient droplet heating, shear effects and internal circulation, and group combustion of droplets.
- Strength: Droplet characterization, measured temperature profiles, qualitative agreement between predicted and measured temperatures. Weaknesses: Lack of gas speed measurements, which are essential for validation, discrepancies between predicted and measured temperatures and inadequate discussions about them, the report does not provide data on the computed droplet velocities and how they (and the model that they are based on) compare to the measure ones. Hence, the Lagrangian droplet model is not validated.
- Yes, the justification for the assumptions regarding the wellbore flow (annular liquid film, with fully developed gas phase flow in the center of the wellbore is well described and is based on data and correlations developed in the literature for wellbore flow. The authors acknowledge the assumptions regarding wellbore conditions and that conditions will change as a function of time. The annular flow assumption and corresponding wall film thickness appear valid for the conditions of the Liberty 90 day WCD conditions.

3.1 Was the physical model for multi-phase flow adequately developed to capture the liquid droplet phase and the gas-phase flow field? Were there any apparent strengths, weaknesses, omissions, or errors? Provide an explanation for your answers.

- Modeling the problem of interest is inherently difficult because of its multiphysics nature. The submodel elements for gas phase (turbulence and combustion), liquid/droplet dynamics, radiation and soot may have been validated independently. However, it is not clear how they perform when coupled like this. There is no discussion of the inherent uncertainty of the combined model. There is limited discussion of the choice or validity of the submodels within the context of the problem of interest. The simplistic nature of these models leaves many constants to either be determined or tweaked to adjust the model predicts to experiments or observations.
- Eulerian Lagrangian formulation is used to model the liquid and gas phases. This is standard practice for large scale applications like the one considered in this study. RANS is used to model the gas phase, while LES would be more accurate, it would also be more expensive. Progress variable approach was used with appropriate closure terms to model the turbulent flame, which is a reasonable approach. Authors could consider performing some higher-fidelity LES to further improve the predictive capability of the simulations to train/improve the RANS modeling approach.
- Strengths: Most of the physical processes have been captured using several sub-models. The model can be computed with reasonable computational cost. Multiphase models are reasonably well tackled. Weakness: The model is primarily developed and validated with lab-scale and medium scale burning. Full-scale wellhead burning may not be accurately captured with the present model. The entrainment model is questionable for wellhead conditions. Omission: In the modeling section, the authors introduced physics-based models to capture various multiphase combustion processes. But, in many instances, they resorted to correlations based on previous studies. The involved multi-scale physics is indeed complicated and difficult to formulate. Such complexity justifies the correlation-based models. However, it is not clear why specific values for model constants were selected. For example, on Page 23 (just before Eq. 33), the authors have taken B0=0.61. Was 0.61 taken from a reference? More importantly, it is also not clear if the values will be different for wellhead conditions. Similar is also true for d_P, F, and \beta concerning Eq. 36 on page 26. Errors: Perhaps a detailed uncertainty analysis is needed to assess the "safety limits" if the model is used for wellhead burning.
- The selection of n-heptane as the single component surrogate fuel for crude oil may be inaccurate in terms of predictions of preferential vaporization, and the resulting gas phase flow field and mixture formation.
- There is concern on the part of this reviewer as to whether the effects of surface tension, viscosity, and volatile range covered by actual crudes are well represented in terms of effects on breakup and atomization of the boundary layer pipe flow. The effects of these parameters along with gas/oil fraction of the crude as well as water content remain to be thoroughly envisioned through the current initial experiments.
- The liquid-phase behavior is basically an input parameter to the computations, and semi-empirical correlations are used to estimate them. A rigorous modeling of the liquid phase is lacking.
- Applicability of RANS based modeling to a multiphase jet needs to be justified. Yet, the model is simple enough, allowing multiple tests and fast outcomes.

3.2 Were the soot and radiation models adequately characterized? Were there any apparent strengths, weaknesses, omissions, or errors? Provide an explanation for your answers.

- If the size and height of the wellhead jet flame is not represented well by the n-heptane surrogate, and the soot characteristics of n-heptane are different than from crude oil this can affect the radiative energy blockage, i.e. the radiant flux by the core gases which can affect the fuel mass consumption rate.

- First, the experiments with n-heptane as the fuel do not well characterize the magnitude of soot yields expected from the lower boiling range of components in crudes and especially those of aromatic structure. Single species experiments with toluene or with mixtures of low boiling point aromatics available from the commercial solvent industry would yield much higher sooting propensity, hence more radiative effects in terms of experimental observations to test radiation effects on burnout efficiency and modeling predictions. Moreover, crudes contain significant fractions of species with boiling points at atmospheric pressure well above 600 C, and that fraction varies substantially by crude source. Those fractions chemically crack in the liquid phase prior to vaporization from spray droplets, eventually yielding cenospheric coke particulates. The particulate mass and number densities will not likely be predicted well for crude conditions by considering only gas-phase sooting contributions, hence not well representing the radiative effects on crude combustion as a function of crude properties. The latter issues may have been viewed as something to be examined in follow on work, but no mention of its likely scale of contribution to model uncertainties is discussed. The more critical issue is that even the gas phase sooting effects were not well tested by experiments involving only n-heptane.
- Even in the simplest of laminar flames, a one-step soot formation model is unlikely to provide a reasonable representation of soot volume fraction and radiation effects. The conditions being modeled here are highly complex. Soot formation will be influenced by turbulence. In addition, droplet formation and evaporation may have a significant impact on soot formation and optical characteristics. At least some attempt should be made to address potential coupling between soot formation/radiation and turbulence, droplet formation/evaporation, and internal mixing of soot and semi-volatile droplets. In addition, there should be some way to validate this part of the model. If nothing else, there should be consistency between the representation of the radiation effects in the model with the emissivity model used in the soot-temperature measurement analysis in which the particles are assumed to be in the Rayleigh regime with an emissivity proportional to $1/\lambda$.

3.3 Were Lagrangian droplet dynamics and thermophysics adequately incorporated into the model? Were there any apparent strengths, weaknesses, omissions, or errors? Provide an explanation for your answers.

- Usual assumption and standard correlations are used in Lagrangian model. The model's capability to simulate denser particle regimes has to be made clear, as EL model is often used for coarser particle laden flows.
- Relevant droplet dynamics are represented through the Lagrangian formulation and sub-models for evaporation, break-up, collisions and coalescence, etc. A single component formulation is assumed for the liquid phase, which in my opinion is not justified. Thermophysical characteristics of a single component will vary significantly from the actual crudes at the well-head. If the actual crude composition was available, it would have been useful to use a surrogate formulation based on the crude composition. The authors have chosen n-heptane since it is one of the components of the crude, but perhaps it is too light to represent crude and hence the sooting characteristics will not be accurate as well.
- In the governing equation for droplet velocity (Newton's law of motion) as well as in the gas-phase equations there is no gravitational (buoyancy) term. One would expect buoyancy to slow the droplet motion in the vertical direction. It is not clear to me why that term is omitted here. For small flames (bench-top), and at high flow rates momentum controls the flow, however, in large scale flames buoyancy will play a critical role in establishing the flow field. Also in the bench-top experiments, a fairly high co-flow surrounding the main fuel-injection tube is used, which prevents buoyant entrainment of ambient air. The report tries to capture the evaporative behavior of a typical crude oil by choosing a single pure n-alkane fuel (n-heptane) as a surrogate. The sooting characteristics, and the thermophysical properties of n-heptane is considerably different for n-heptane compared to crude oil. Other phenomena, such as preferential evaporation and swelling need to be

incorporated in the future work. The "d-square" type single- component evaporation model is certainly inadequate for crude oil evaporation. The authors do state that they are planning to model a typical crude oil at a later stage.

- Again, transient heating of droplet, internal circulation, and group combustion were not considered.
- Strength: Attempt to include thermal and dynamic effects. Weakness: Adequacy of the drag model is questionable. The model was not validated or compared to data.
- An Eulerian Lagrangian approach was used for the gas and droplets, which is fine. The soot and droplet models (and others) include the relevant formation and oxidation mechanisms; however, the models are semi-empirical and were not developed or tested for oil well fires, so there is likely a high level of uncertainty. The models are adequately described or referenced; however, the applicability is not always well documented, e.g., the droplet breakup model was developed for flow in a pipe. Is it appropriate for Liberty oil and gas conditions? The combination of several semi-empirical models without a sensitivity analysis to understand the impact of the modeling approaches and input parameters is a significant weakness.

4. Does the droplet injection model adequately simulate realistic diameters and velocities of two-phase, high-speed flows that would occur during a wellhead blowout event? Were there any apparent strengths, weaknesses, omissions, or errors? Provide an explanation for your answers.

- A simplified droplet injection model is used that takes care of droplet stripping and liquid-sheet breakup through correlations. Secondary breakup, droplet dynamics and deformations are not included due to the complexities. For the gross data modelled, these should be fine.
- The experiments and simulations were performed under significantly scaled down conditions. It is unclear if the droplet diameters and velocities considered under the lab-scale flames will mimic the actual well-head. Depending of the Weber numbers in the actual well-head, droplets may be in different break-up regimes than the ones considered in the lab scale tests. In the absence of experimental data inside the pipe and injection plane, the authors have made certain assumptions, and have clearly stated them. In the reviewers' humble opinion, the authors have been very transparent in their approach and assumptions. Without sufficient data about the pipe flow and injection conditions, it is very difficult to initiate the spray flame simulations using the droplet injection model. KH instability is assumed to be the primary aerodynamic break-up mechanism. However, there could be significant cross-flow/gust of air which may result in different dominant breakup mechanisms such as those encountered in gas turbines (jet in cross flows).
- Strengths: Most of the physical models are in place. Weakness: The breakup models are questionable under the wellhead condition. In particular, the authors commented that the compressibility effect would be vital in certain flow conditions. The used KH-type breakup model may not be sufficient enough under such conditions. Omission: The rationale behind some of the model constants was not discussed. (e.g. see between Eqns 37 and 38 in page 27). Detailed simulation of intermediate-scale burning has not been done. Errors: Perhaps a detailed uncertainty analysis is needed to assess the "safety limits" if the model is used for wellhead burning.
- The drop injection model may not adequately simulate particle mean diameter and size distributions in a two-phase high speed flow. In a wellhead blowout event, there may exist cross flow winds that would modify the entrainment patterns and droplet size distributions.
- My opinion is that extrapolating the experimental efforts to the scale of the actual problem of interest remains an unknown at this point, especially considering the limited information presently acquired on the effects of crude surface tension viscosity, gas/oil fraction, and boiling range of components, particularly the heavier component fractions and their aromaticity.
- Here, reference is assumed to be on the initial size and velocity, not the predicted values in time.

- The authors attempt to introduce a realistic phenomenological model of the multiphase. The adequacy of this model needs to be validated/proven. The relevance to the full scale system is questionable
- This part of the model seems largely conjecture, which is understandable considering the lack of information to support developing a droplet injection process for a well bore blowout. I did not see a lot of data comparing the model results to wellhead blowout events.

5. Does the validation process capture the controlling physical properties to a sufficient level of accuracy including transport and boundary conditions at the bench- and intermediate-scales for both gas-phase and two-phase turbulent spray? Were there any apparent strengths, weaknesses, omissions, or errors? Provide an explanation for your answers.

- The experiments provide a very nice database for further model development and a starting point to implement a more realistic choice of fuels that mimic the performance of crude oil. However, and given the above comments, it is not clear to the reviewer based on the limited validation data whether the models are adequate or not. Also, it would have been helpful to read information about the scope of the CFD predictions. Are they designed to predict the experiments or the actual wellhead burning scenarios within prescribed error bar or simply predict trends (e.g. what happens if the discharge rate is increased or decreased)? Addressing this question could have provided a better appreciation of the value of the CFD modeling and whether higher fidelity modeling approaches are needed.
- I think that the sequence of the experiments that were described was logical. The authors first investigated as gas phase flame (GPF) with a propane jet in a vitiated co-flow provided by a lean premixed hydrogen/air flame. They then progressed to a two-phase jet with “bench-scale spray flame” (BSSF) with a gas phase flow of ethane and liquid injection of heptane. The BSSF flow conditions were configured such that the system was in the annular flow regime. Finally they investigated an intermediate scale experiment (ISE) with gas flows of methane and propane and a liquid flow of crude oil. The progression from very fundamental flames to a flame with crude oil injection has the advantages of providing validation data for the models that are being developed and gaining confidence both in the modeling and the experimental techniques on the GPF and BSSF systems before moving on to an investigation of the ISE.
- The validation of bench scale study in terms of comparison of measured and predicted temperatures has been reported. There are discrepancies, however, the overall agreement seems to be satisfactory. Intermediate scale results from experiments are shown, but not an explicit comparison with prediction. For several measurements made, few more parametric validations could have been done.
- While the reviewer is not an expert, the authors have done a good job in coming up with a detailed experimental campaign with well-established boundary conditions in the experiments.
- The quantitative validation between experimental and simulation is somewhat limited. Only temperature fields were validated, which show reasonably good agreement.
- See my above discussions with regard to the limited range properties and choice of a low shooting propensity liquid fuel for evaluating radiation loss contributions to combustion burnout efficiency.
- The bench-scale experiment uses a very small injection tube (less than 1 mm) and it is clearly not a model for capturing oil well blowout scenarios. However, it can be used to validate general turbulent-jet flames with dispersed droplets – a problem reasonably well understood. The intermediate-scale experiment still has a fuel injection tube diameter of 0.25”, still small compared to real wellhead configuration and scaling of these results to wellhead fires are difficult, particularly with regard to radiation.
- This is not my expertise, but I had a related question. I am unclear on how the scaling from the WCD model was done to bench and intermediate scale initial and boundary conditions.

- The validation process neglects soot abundance measurements, which is very important for validating the soot formation model and soot radiation effects.
- Weaknesses: 1. Lack of gas velocity measurements prevents validation of the basic RANS tool. 2. Limited resolution of the back-illuminating imaging system. 3. The report does not provide a comparison between the PDA and imaging results. 4. There is no comparison between the modeled and measured droplet behavior.
- Heptane properties were used for the liquid phase of the model. However, oil is a blend of heavier and lighter components. I expect this assumption to be quite impactful on the droplet dynamics, e.g., evaporation rates, droplet diameter, etc. The assumption of a single component liquid is likely a weakness of the model, but it is unclear on how significant the impact is without sensitivity analysis. How was the stagnation pressure selected for the exit plane of the well head? The rationale for the progression from the lab scale modeling and experiments to the actual well bore conditions is not well explained or justified. What scaling relationships are assumed?

6. Were the phase doppler anemometry and diffuse back-light illumination imaging diagnostic methods (6.1 and 6.2 below) for the droplet behavior measurements appropriately designed, clearly described, and adequate to capture droplet behavior for the Gas Phase and Two-Phase Spray Flame? Were there any apparent strengths, weaknesses, omissions, or errors? Provide an explanation for your answers.

6.1 Phase Doppler Anemometry

- The phase Doppler anemometry (PDA) experimental system was described well and the experiments appear to have been performed in a very competent manner. The system included two PDA systems, one for measuring velocities in the x- and z- directions (this system used 660-nm and 785-nm beams) , and one for measuring velocities in the y-direction (this system used 632-nm beams. The system used information from all three beam crossings to determine droplet size. This is a more sophisticated system than a PDA system I have used which has only two wavelengths.
- More details on uncertainty analysis should be useful.
- The technique utilized, experimental arrangements etc. are adequately described. A couple of comments regarding the interpretation of the data: (1) Page 61(under Fig. 32), it was commented that outside r=+/-4mm, no droplets were observed. However, measurements were provided beyond this radius e.g. Fig. 32). (2) Page 62 last sentence: Authors stated, "..so there is likely a slight increase in ethane density….". One should note that a change in spray cone angle will also change the mean velocity.
- Where it can be implemented, PDA is adequate. However, it has a limited range.
- The diagnostic methods were well described.

6.2 Diffuse Back-Illumination Imaging

- The diffuse back-illumination imaging (DBI) results were crucial for qualitative understanding of the structure of the liquid flow in the two-phase system and for proper interpretation of the PDA measurements. The type of information obtained from the DBI measurements as shown in Figs. 38 and 39 provides a great deal of insight into the flow structure. The reason why PDA measurements could not be performed near the tube exit becomes perfectly clear upon examination of these figures. The time-dependent behavior as revealed by the high-speed DBI measurements shown in Fig. 39 was very interesting.
- The technique utilized, experimental arrangements etc. are adequately described. The extensive postprocessing analyses of the data set taken are still pending. The approach does show initial promise.

- The high-speed back-illuminated imaging does provide sufficient information to study the droplet dynamics. Only preliminary results are provided and the detailed analysis is left to future investigations.
- A difficult measurement to perform, analysis based on thresholded images raises questions about accuracy. Although mentioned as a possibility, the authors did not measure the droplet velocity from the images.
- This section in general is not written well, with repetitions and is missing an uncertainty analysis, accuracy and precision information. Additionally, issues of volumetric versus planar measurements and phenomena are not discussed.

7. Were the diagnostic methods (7.1 and 7.2 below) for the temperature measurements appropriately designed, clearly described, and adequate to capture temperature for the Gas Phase and Two-Phase Spray Flame? Were there any apparent strengths, weaknesses, omissions, or errors? Provide an explanation for your answers.

7.1 Coherent Anti-Stokes Raman Spectrometry-based Thermometry (CARS)

- The CARS temperature measurements have been performed in a competent manner. I am somewhat concerned that the average temperatures that were reported were determined from averaged CARS spectra; the CARS spectra were average for 300 to 500 shots for the gas-phase flames, for example. In a gas flow with significant temperature fluctuations due to turbulence, the temperature determined from an averaged CARS spectrum will be biased towards lower temperatures because CARS signals will be stronger from the higher density, lower temperature gases. In extreme cases with very significant temperature fluctuations it will not be possible to extract an average temperature from an averaged CARS spectrum because it will not be possible to fit a theoretical single-temperature spectrum to the averaged CARS spectrum. For the spectra shown by the authors this does not seem to be the case, it appears the temperature fluctuations were not that severe. However, the rigorous way to analyze the CARS data is to fit the single-shot CARS spectra and then to determine the average temperature from the average of the single-shot temperatures. There are two disadvantages to this more rigorous approach. The first is that the single-shot spectra are noisier than the averaged spectra and thus are more difficult to fit. The authors did not show any single-shot spectra so the quality (SNR) of the single-shot spectra is hard to evaluate. The authors do indicate on page 153 that "The signal-to-noise ratio in the CARS spectra for some of the conditions in Table 4 was sufficient to perform a shot-to-shot analysis of the distribution in temperature." I believe that the authors are trying to show the comparison of the average temperature determined from the single-shot spectra analysis and the averaged spectrum analysis in Fig. 53. I believe that the open circles in Fig. 53 are the average temperature determined from the averaged CARS spectrum although this is not explicitly stated and the open circles are labeled "Measurement." The second disadvantage is that it takes much longer to fit 300 to 500 single-shot spectra than a single averaged spectrum. The fitting time can be reduced with library fitting routines, but considerable expertise is required to develop the required computational framework. However, for future CARS measurements in this group, it is essential to further develop the computational framework for analysis of single-shot CARS spectra.
- The temperature data obtained here can be used to draw logical conclusions in a relative manner on various parameters.
- There is an odd mix of really detailed (and somewhat superfluous) information and lack of specifics in the CARS section of the report. What are the uncertainties and error bars associated with fitting the CARS spectra? The comparison of temperature data (e.g., Fig. 28, Fig 30, etc.) is meaningless without error bars. Fig 45 includes error bars, but does not define their origin.

7.2 3-Color High-Speed Pyrometry

- I am much less familiar with the color high-speed pyrometry (CHSP) technology. The assumption of inverse dependence of the emissivity on wavelength is reasonable, and the rough agreement of the CARS and CHSP temperatures in the BSSF tests is encouraging. CHSP as pointed out by the authors is much easier to apply than CARS and it is much easier to obtain very high data rates. CHSP temperatures must always be regarded somewhat skeptically because of the path averaged nature of the measurement. The authors also point out difficulties due to the optically dense nature of the intermediate scale flames.
- The temperature data obtained here can be used to draw logical conclusions in a relative manner on various parameters.
- The 3CHIP method for temperature analysis of soot has some issues, as does the interpretation of the results. First, the emissivity of soot changes dramatically with maturity. Lower in the flame, where the soot is less mature, the dispersion exponent will be much larger the one, i.e., the emissivity is proportional to $1/\lambda^{\xi}$, where $\xi >> 1$ for young soot. Using a value of ξ that is too small will lead to an overprediction of the temperature. Soot will age and mature with increasing height in the flame. In normal diffusion flames, soot is also often more mature at the flame front at higher radial distances. At full maturity, the dispersion exponent is less than one ($\xi < 1$), and using the value of unity, will lead to an underprediction in temperature. Thus, the trend in temperature may be the opposite of that suggested in Fig. 30 for the particulates as a function of height in the flame, consider the change in optical properties with soot maturity. Along the edges of the flame, optical dispersion effects may highly perturb the 3CHIP measurements because of the refractive index changes with temperature. Finally, it is highly unlikely that soot will have a different temperature from the gas phase at atmospheric pressure because conductive heat transfer equilibrates temperatures on timescales of nanoseconds at such pressures. In addition, if there are interactions between less volatile crude oil and soot particles, optical properties of the internally mixed particles will deviate from those of mature soot and look more similar to young soot, leading to larger deviations from a $1/\lambda$ dependence of the emissivity and significant errors in inferred temperatures. Furthermore, for high-sooting conditions, luminosity measurements need to be corrected for reabsorption.
- The data is qualitative at best.
- See last comment on CARS measurements. No uncertainties or standard deviation data are reported to define accuracy or uncertainties of the pyrometry measurements.

8.1 Do the results adequately characterize evidence of the droplet characteristics including droplet breakup, the droplet size (diameter), droplet speed, and the duration of droplet in fire (bench- and intermediate-scales)? Were there any apparent strengths, weaknesses, omissions, or errors? Provide an explanation for your answers.

- The answer is yes for the bench-scale spray flames due to the PDA and DBI measurements. However, it does not appear that these techniques were applied to the intermediate scale flames.
- Only droplets' SMD distributions are presented in detail. Results on droplet speed, droplet break-up, heterogeneous combustion etc., have not been reported.
- The benchtop experiments have provided detailed measurements of film breakup, atomization etc. However, it is not clear if such insights can directly be translated to the wellhead burning. The wellhead flow conditions, pressures etc., are different and may not exhibit similar breakup dynamics. Modeling and simulation, on the other hand, did not provide microscale/ droplet-level information. As such, it is not possible to judge if it predicts the conditions beyond the validated range.

- The high speed backlit imaging of the droplet provides sufficient data on droplet dynamics. In this report no direct comparison between the experiments and the simulation are shown. Future studies should address this.
- The experimental data, e.g. the droplet size distributions are presented, but are not used for evaluating the droplet models at all.
- No, most of these parameters were not considered in the report descriptions of the experiments and modeling.

8.2 Does the research product accurately expand predictions of droplet diameters beyond current limited validated ranges? Were there any apparent strengths, weaknesses, omissions, or errors? Provide an explanation for your answers.

- There is no clear discussion of this in the report.
- Accurate measurements of droplet diameters are extremely challenging and authors have performed a thorough experimental campaign. It would have been useful to have error bars in their measurements. Fig 34 a, at Z=10 mm, Eth 0.2/Hept 0.4 measurement does seem to show a weird spike at the center line. The reason for this behavior was not explained.
- The range of experimental characterization, the liquids were chosen to be used in the evaluation, in my opinion, limit the extrapolation of results to the scales required for application.
- The authors point out how the high speed images can be further analyzed to extract the underlying physics of the processes involved.
- Scaling trends are hardly discussed.
- No, most of these parameters were not considered in the report descriptions of the experiments and modeling.

9. Does the research product accurately characterize the impact of two-phase flow regimes (bubble, slug, and churn) on the effluent plume (bench- and intermediate-scales)? Were there any apparent strengths, weaknesses, omissions, or errors? Provide an explanation for your answers.

- The answer is not an absolute NO; but, it may be difficult from the experimental standpoint to capture this impact.
- Bench scale temperature data has been validated. Intermediate scale data needs validation. Data on gas-phase are sufficient. More work is required to reveal two-phase characteristics. Demonstration of the numerical model with EL approach to reveal the two-phase aspects has not been explicitly done as validation is shown in terms of temperature data.
- For the simulations, authors assume annular-mist flow behavior for the sake of brevity and applicability as these sprays probably atomize well. Based on the experimental conditions in table 5, the reviewer is unable to determine the two-phase flow regime in the bench and intermediate scales.
- Yes. The model will work within the range over which the correlations sub-models are valid. However, a big concern is if those models will work for actual well-head burning conditions. A detailed uncertainty analysis perhaps is needed. I would defer this point to other committee members who have more experience in this particular area.
- The impact of two-phase flow regimes on the effluent plume is not addressed in detail. Only annular-mist flow regime is considered aligned based on WCD output results for the Liberty Project.
- It appears that the authors explicitly state that bubble, slug, and churn regimes are not addressed for the sake of brevity. On P 77, they state "it is unclear what kind of flow structures form when bubbly, plug, or churn flows are expelled through a wellhead. It is reasonable to assume that these lower velocity flows are more likely to form pools or fountains than well-atomized sprays.

Therefore, for the sake of brevity and applicability, we will focus on the annular-mist flow behavior."

- This was not clearly explained
- These flow regimes are extremely difficult to model, and the report does not provide any evidence that they are accounted for adequately
- I don't believe the different flow regimes were considered in the modeling approach? Only misty flow. In the experiments, again, I believe only one regime was considered and it is not clear which regime it was.

10. Does the research product adequately address how the wellbore flow would influence the ejected spray plume behavior, which directly influences how the oil and gas burns and how much will either fall back to the surface or remain vapor? Were there any apparent strengths, weaknesses, omissions, or errors? Explain your answers.

- The answer is not an absolute NO. The authors did establish that the worst case spill scenario does not correspond to a high discharge rate. However, it is not clear that accounting for real wellhead conditions and crude oil properties and burning behavior has been adequately addressed to extrapolate this trend from experiment to wellhead conditions.
- As the real process is quite complex, the approach here has been to use surrogate liquid as well as gas fuels. Obviously, n-heptane will not reveal the characteristics of the crude oil. The droplet formation and its dynamics can be quite different. Thus, burn efficiency data may not be extrapolatable.
- Several assumptions were made regarding the flow conditions inside the pipe. While in bench and intermediate scale experiments, there was evidence that fallout of large droplets at the periphery of the plume, falls back to the surface, resulting in reduced burn efficiency, it is unclear if simulations actually captured this trend. The connection between pipe flow and ejected spray plume behavior is weak. The only way to improve this connection will be to perform detailed simulations of the pipe flow under different conditions and use the simulations as boundary conditions for the corresponding Eulerian-Lagrangian simulations. In the absence of multi-phase diagnostics within the pipe flow or simulations, the semi-empirical correlations are not sufficient to describe the spray flame behavior.
- The report does not provide detailed information on the fraction of fuel being burned vs. aerosolized vs. deposited/settled due to gravity. A proper estimation of these numbers will be difficult to evaluate for the wellhead conditions from the benchtop or intermediate-scale experiments, in the reviewer's opinion.
- The CFD model has considerable uncertainty in its components which have not been characterized. Assumptions for the combustion model based on a single progress variable and presumed shape pdf for the partially premixed flames based on marginal pdfs for the 2 mixture fractions and progress variable have not been validated. The coherent flame model also has a lot of tunable constants. It is unclear which submodel affects the burning rate the most without some sort of sensitivity or UQ analysis.
- I do not believe that the current cursory work which in the authors' opinions was to initiate the process of building a predictive tool is sufficiently advanced in either development or experimental testing to answer this question.
- Wellbore flow or WCD modeling is not detailed or provided (Appendix G), and it is difficult to know the uncertainties associated with the results which are down-scaled for input into the bench-scale problems. The Hilcorp report includes some reservoir rock and fluid properties (section 4), and well design (section 8) amongst other data that can be used along with analog and dynamic data as available to build an independent WCD model to verify output or to cross-validate WCD output amongst different wellbore flow modeling methods. The Endicott reservoir (Ali et al., 1994)

could be used as analog. This would help provide confidence to the WCD work, and the output thereof. A related question is also the impact of wellbore modeling method on the two-phase flow characterization at the wellhead, used as input to study at hand.

- The attempt to explore scaling trends is commendable. The results and comparisons are limited. Relevance to full scale system is questionable.
- The report does include a strong foundation of modeling and experimental studies of some of the physical and chemical mechanisms relevant to wellbore ignition and combustion, but the effects of wellbore flow are not considered in a broad way. Similarly, the sources of combustion inefficiency are only identified in a general way, lacking quantitative measurements over a robust range of conditions, and/or justification for the limited conditions studied.

11. Does the research product accurately predict the length of fire plume, location of flame anchoring, height of flame, width/angle, expansion, etc.? Were there any apparent strengths, weaknesses, omissions, or errors? Explain your answers.

- This is not an absolute YES. The authors could have made their comparisons clearer by using tables reporting the different quantities and by presenting the results of the computational and experimental studies in one section. The second issue is the interpretation of what "accurately" means. The authors claim consistency in trends and values; but, a quantification of the compared values is certainly better.
- The gas-phase overall features can be satisfactorily understood. Apart from the gross features, droplet dynamics, heterogeneous droplet flames etc. require more work.
- For Propane fuel, these parameters are reasonably well predicted, but results with the surrogate fuel assumed (heptane), are not presented. While the simulations can capture reasonable trends, quantitative values of temperature profiles at different locations upstream and downstream locations of the flame lift-off length for different propone flow rates are not well captured. Capturing flame lift-off length, height, size etc. has been a challenge for the spray-flame community for decades, especially for high co-flow conditions. While there may be several reasons for this mis-match, the reviewer believes that the two-phase flow mixture at the pipe flow exist needs to be better characterized to initialize the spray flame more accurately. The choice of turbulence model is also known to be important and the reviewer expects that LES would do a better job.
- The modeling may not be predictive due the many assumptions made, and the lack of understanding of the sensitivity of the characterization of the plume (burning rate, height, flame lift off, spread angle,etc) to the many model assumptions. For example, are f1, f2, c, and H_bar statistically independent such that product of the independent pdfs is the same as their joint pdfs? The laminar flame speed model used in the source term for the progress variable is questionable as it is based on tabulated high-temperature propane-air mixture flame speeds which may not be representative of the flame speed correlations of the mixtures of well gases and volatile oil species over the range of conditions encountered in the wellhead. It is also uncertain whether the normal flame propagation term P4 in the extended coherent model accounts for flame stretch correlations. It seems that the submodels needed to be better validated individually, before being validated collectively.
- I do not believe that the current cursory work which in the authors' opinions was to initiate the process of building a predictive tool is sufficiently advanced in either development or experimental testing to answer this question.
- Only qualitative trends are provided. For the bench-scale model a co-flow of water vapor, oxygen, and nitrogen at 1400 k with an axial flow velocity of 2 m/s is specified. The authors note that the flame cannot be stabilized without this co-flow. This leads to a question, if a stable burning configuration is even possible when the gas flow rates are high in a real situation. Perhaps an upper limit to the well-gas velocity should be calculated and presented as one of the worst case scenarios.

For the intermediate-scale model the domain vertical size is truncated at 2.5 m and the flame extends past this value, and no direct comparisons are possible.

- The theory for the two-phase flow has not been fully utilized.
- The report does not provide a comparison between the measured and modeled plume length, etc.
- The model may predict these characteristics, but the simulations were not quantitatively or qualitatively validated for all these metrics.

12. Does the research product determine the primary mechanism driving burn efficiency?

- The research product highlights and provides critical details of the physical processes underlying the wellhead burning. However, the multi-scale, multi-physics problems are difficult to tackle effectively. Thus, the efforts of the present research were intentionally kept in understanding the physics in lab-scale or intermediate-scale experiments, which allowed them to validate the developed numerical models at least in a qualitative sense. In that way, the research does provide critical information on primary mechanisms of wellhead burning. However, one should also be careful in extending these results directly in wellhead conditions where the flow parameters, the fuel characteristics, well-hear pressure can be significantly different, leading to very different burn efficiency.
- The authors conclude that the annular fluid film that escapes the injection tube without being entrained into the main flow is the primary cause driving the burn efficiency. But this conclusion seems to be limited to the worst case scenario of lower gas flow rate postulated in the study. At high gas flow rates it may not be possible to intentionally ignite the oil/gas jet.
- A clear explanation was not seen
- No, not without sensitivity analysis of the sub-models used in the overall modeling.

13.1 Were the conclusions based on the OSRR 1063 study findings in the report logical and appropriate based on the results? What other conclusions related to the study were made and are appropriate?

- Note that the Yes response is made related to the studies presented in the report. It is not clear if a strong case is made to extrapolate the conclusions to wellhead burning.
- As mentioned earlier, the data from this study can form validation data for a numerical model. The model can also be improved upon several aspects. Conclusions about actual scale scenario cannot be drawn within this study.
- In the “executive summary” the authors’ claim that with the CFD tool that has been established (based on bench and intermediate scale experiments), if the characteristics of the well (e.g., mass flow rate and oil properties) are known, fall out fractions can be estimated. In reviewers’ opinion this claim may not be substantiated since even for a single component bench scale experiments, simulations do not capture the flame characteristics very well. While the procedure may be transferable, the model is not robust enough to mimic a well-head where there may be other physical factors affecting the spray flame. The intermediate scale experiment provides a way to estimate the burn efficiency. However, the experiments are performed under well controlled conditions and assuming certain pipe flow regime. It is unclear if the burn efficiency methodology is transferable either.
- Future work is needed to address the physical and chemical properties of more representative crude oil surrogates in the modeling effort. The experiments identified mechanisms for reduced burn efficiency due to the fall out of large droplets formed at the periphery of the plume from the unentrained film of the wellbore flow.
- I answer yes above, but the conclusions themselves are very limited in value in terms of assessing the adequacy of the current first-order modeling conceptualization to address the issue of

predictively modeling combustion efficiency well for various well-head geometries, flow rates, and crude properties.

- The main conclusion seems to be that the liquid film that forms on the periphery of the plume is the major cause of lowering the burn efficiency.
- Seem reasonable (although CFD is not my area of expertise, and so this comment is general). Impact of different flow regimes through time (for wellbore) could be included/expanded.
- As the conclusions indicate, the study is not complete. The scope of the validation is limited to temperature measurements, the modeled and measured droplet statistics are not compared, the gas velocity is not measured, the droplet velocities are partially measured, the plume scales are not compared.
- Given the objective of the report was to define burn efficiency of the wellhead flow, it seems imperative to include the details on the burn efficiency measurements in the body of the report, and not as an appendix. Conversely, the secondary considerations (turbulence features) could be relegated to an appendix along with the lengthy descriptions of diagnostic details. Instead the diagnostic sections should include descriptions of rigorous uncertainty and repeatability analysis of the experimental methods. The conclusion about droplet fallout contributing significantly to low combustion efficiency at lower wellhead flows is important, but needs validation and discussion in terms of scaling to an actual wellhead.

13.2 Are there any additional study findings or conclusions that could be drawn from the study? Provide an explanation for your answers.

- This study is an excellent first step and in fact motivates both additional experimental and computational studies. Also getting more field data on the well-head and crude oil characteristics will be extremely useful next steps.
- A significant conclusion as regards the computational model is the need for full coupling between the gas and liquid phases, their thermodynamics and chemistry such that their momentum, energy, mass transport and reaction are coupled. Further analysis of the assumptions made in the various submodels quantifying their accuracy is needed. Better understanding of the propagation of uncertainties and sensitivities of the plume parameters to the various modeling assumptions is needed.
- I believe it would be important to have more elaboration as to the basis in the first-order model conceptualization, a discussion of what the next steps in revising it should be, and what additional submodel considerations need to be significantly refined to consider full range crude property effects on combustion efficiency at full-scale conditions.
- The experimentally observed oscillations of the fire plume seems noteworthy and deserves further analysis. The feasibility of developing a computational model to study oil wellhead fires is demonstrated, though in a limited range of conditions. Future improvements are warranted.

Appendix C

Peer Review Schedule and Committee Meeting Summaries

Project Schedule and Timeline	
Month	**Activities and Milestones**
November 2020	• Contract awarded and project start
December 2020	• Sponsor orientation and launch meeting • Draft peer review charge document • Dissemination of Call for Nominations
January-February 2021	• Committee selection process • Government Orientation Meeting • Documentation of the Peer Review Selection Process
March 2021	• Review of proposal begins o Prepare the Peer Review Materials o Manage the Peer Review Process • Provide draft charge document to committee • Peer Review Meeting 1
April 2021	• Collect and compile committee comments on review questions • Peer Review Meeting 2 • Peer Review Meeting 3
May-July 2021	• Peer Review Meeting 4 • Revise and finalize consensus findings and conclusions • Complete report draft • Complete National Academies Report Review Committee process • Finalize report, deliver to BSEE, public release
August 2021	• Publish NAS Consensus Report • Government Follow-up Meeting
September-November 2021	• Dissemination activities • Close out of the contract

Committee Meeting Summaries

Peer Review Meeting 1

March 26, 2021

Closed meeting of the committee to conduct the bias and conflict of interest discussion. Academies' staff led a discussion with the committee to address potential biases and conflicts of interests and to allow the committee opportunity to determine if it is appropriately constituted to address their Statement of Task.

Peer Review Meeting 2
April 6, 2021

The committee first met in closed session to discuss their Statement of Task, the charge questions provided to the committee by the project sponsor, and the project schedule. The committee then entered an open session to meet with the project sponsors and the authors of the interim report to ask relevant questions to provide clarity on their task.

Peer Review Meeting 3
April 21, 2021

The committee heard from the authors of the interim report to ask additional questions in open session. The meeting was also open to pre-registered members of the public for comments.

Peer Review Meeting 4
May 12-13, 2021

During a two-day closed session meeting, the committee finalized their conclusions and recommendations, came to consensus on their responses to the provided charge questions, and finalized drafting the report.

Appendix D

Additional Resources

Worst Case Discharge/Wellhead Modeling

Bureau of Ocean Energy Management. Regulatory Analysis. Webpage. https://www.boem.gov/oil-gas-energy/resource-evaluation/regulatory-analysis.

Society of Petroleum Engineers. 2015. Calculation of Worst-Case Discharge (WCD). SPE Technical Report Rev. 1.

Teles, F. B. X., P. J. Waltrich, I. Gupta, R. Hughes, M. S. Capovilla, and F. A. V. Cordoba. 2018. Development and Improvement of Flow Models Applied to Multiphase Flows in Large-Diameter Pipes and High-Velocity Flows. Bureau of Ocean Energy Management, US Department of the Interior M17PX00030.

Waltrich, P. J., M. S. Capovilla, W. Lee, P. C. de Sousa, M. Zulqarnain, R. Hughes, M. Tyagi, W. Williams, S. Kam, A. Archer, J. Singh, H. Nguyen, J. Duhon, and C. Griffith. 2019. Experimental Evaluation of Wellbore Flow Models Applied to Worst-Case-Discharge Calculations for Oil Wells. SPE Drill & Compl 34 (03):315–333. doi: https://doi.org/10.2118/184444-PA.

Droplet and Spray Behavior

Sirignano, W. A. 2012. Fluid Dynamics and Transport of Droplets and Sprays: Second Edition. Cambridge: Cambridge University Press.

Particulate Emissions

Kwon, H., S. Shabnam, A.C.T. van Duin, and Y. Xuan. 2020. Numerical simulations of yield-based sooting tendencies of aromatic fuels using ReaxFF molecular dynamics. Fuel 262:116545.

Lautenbergera, C. W., J. L.de Risb, N. A. Dembseya, J. R. Barnetta, andH. R. Baumc. 2005. A simplified model for soot formation and oxidation in CFD simulation of non-premixed hydrocarbon flames. Fire Safety Journal 40 (2):141-176.

Rangwala, A. S. and X. Shi. 2016. Burning Behavior of Oil in Ice Cavities: Final Report. Bureau of Safety and Environmental Enforcement, US Department of the Interior E14PC00010.

Water and Crude Oil

Erua, E. 2015. Impact of Water Content in Hydrocarbons using Consequence Modelling. IChemE Symposium Series 160.

Crude Oil Properties and Surrogates

Hollebone, B. 2015. The oil properties data appendix. Pp. 577-681 in Handbook of Oil Spill Science and Technology, M. Fingas, ed. New York: John Wiley and Sons Inc.

Urban, D.L., S.P. Huey, and F.L. Dryer. 1992. Evaluation of the coke formation potential of residual fuel oils. Symposium (International) on Combustion 24 (1):1357-1364.

Won, S.H., S.J. Lim, S. Nates, A.K. Alwahaibi, F.L. Dryer, F. Farid, and M. Hase. 2021. Combustion characteristics of crude oils for gas turbine applications by DCN measurements and NMR spectroscopy. Proceedings of the Combustion Institute 38 (4):5463-5473.

Appendix E

Biographical Information of Committee Members

Margaret Wooldridge (Chair) is an Arthur F. Thurnau professor in the departments of mechanical engineering and aerospace engineering, and director of the Dow Sustainability Fellows Program at the University of Michigan. Her research program spans diverse areas where high-temperature chemically reacting systems are critical, including power and propulsion systems, fuel chemistry, and synthesis methods for advanced nanostructured materials. Her research team has pioneered methods for characterizing fundamental fuel properties and performance in modern spark-ignition and gas-turbine engines. Dr. Wooldridge served on the faculty at Texas A&M University in 1995 before joining the University of Michigan in 1998. She is a 2013 recipient of the Department of Energy Ernest Orlando Lawrence Award and a fellow of the Combustion Institute, the American Society of Mechanical Engineers, and the Society of Automotive Engineers. Dr. Wooldridge received a PhD in mechanical engineering from Stanford University.

Jacqueline H. Chen, NAE, is a senior scientist at the Combustion Research Facility at Sandia National Laboratories. She has contributed broadly to research in turbulent combustion, elucidating turbulence–chemistry interactions in combustion through direct numerical simulations (DNS). With the goal of achieving scalable performance of DNS on heterogeneous computer architectures, Dr. Chen leads an interdisciplinary team of computer scientists, applied mathematicians, and computational scientists to develop exascale DNS capability for turbulent combustion with complex chemistry and multiphysics. Dr. Chen is a fellow of the Combustion Institute and the American Physical Society, and an associate fellow of the American Institute of Aeronautics and Astronautics. She received the Combustion Institute's Bernard Lewis Gold Medal Award in 2018, the Society of Women Engineers Achievement Award in 2018, the Department of Energy Office of Science Distinguished Scientists Fellow Award in 2020, and the R&D 100 Award for the Legion Programming System in 2020. Dr. Chen was elected to the National Academy of Engineering in 2018. Dr. Chen served on the National Research Council Committee on Building Cyberinfrastructure for Combustion Science. She received a PhD in mechanical engineering from Stanford University.

Frederick L. Dryer, NAE, is an Educational Foundation distinguished research professor in mechanical engineering at the University of South Carolina. He was previously a professor of mechanical and aerospace engineering at Princeton University. Dr. Dryer's research expertise spans a wide range of areas, including thermodynamics; physical chemistry; chemical kinetics; fluid dynamics; heat transfer; abatement of unwanted emissions from energy conversion systems; and understanding and mitigating fire hazards associated with the use of gaseous, liquid, and solid materials on earth and in low-gravity environments. He is a current fellow of the Combustion Institute, a former associate editor and editorial board member of *Combustion Science and Technology*, and a former editorial board member of the *International Journal of Chemical Kinetics* and *Progress in Energy and Combustion Science*. Dr. Dryer was elected to the National Academy of Engineering in 2021. He received a PhD in aerospace and mechanical sciences from Princeton University.

Tarek Echekki is a professor in the Department of Mechanical and Aerospace Engineering at North Carolina State University (NCSU). He is an expert on computational combustion and the modeling and simulation of turbulent combustion flows. Prior to joining NSCU in 2002, Dr. Echekki worked at the French

Petroleum Institute; Sandia National Laboratories; and the University of California, Berkeley. He is a fellow of the American Society of Mechanical Engineers (ASME) and an associate fellow of the American Institute of Aeronautics and Astronautics. Dr. Echekki serves presently as associate editor for the ASME *Journal of Heat and Mass Transfer*. He has served on many panels in the past associated with grant proposals at the National Science Foundation, the U.S. Department of Energy, and the German Research Foundation, in addition to serving as a frequent reviewer for proposals and publications. Dr. Echekki received a PhD in mechanical engineering from Stanford University.

Ipsita Gupta is assistant professor in the Craft and Hawkins Department of Petroleum Engineering at Louisiana State University. She conducts research on multiscale, multiphysics problems using coupled fluid and heat flow, and reactive transport modeling for wellbore integrity, reservoir characterization, and gas hydrates. She has also conducted Bureau of Ocean Energy Management–sponsored research on worst-case discharge modeling from well blowouts. Dr. Gupta's industry experience at Chevron spans strategic research and technology development in carbonate reservoirs, including those in Partitioned Zones, such as the Wafra oil field, and technical services and large capital project maturation in the Gulf of Mexico. She is a recipient of federal and industry grants, and the 2018 National Academies of Sciences, Engineering, and Medicine Gulf Research Program (GRP) Early Career Research Fellowship. She is coprincipal investigator on the National Academies GRP Safer Offshore Energy Systems grant "Mitigating Risks to Hydrocarbon Release Through Integrative Advanced Materials for Wellbore Plugging and Remediation." She received a PhD in geological sciences from the University of South Carolina.

Joseph Katz, NAE, is William F. Ward Sr. distinguished professor of engineering and director and cofounder of the Center for Environmental and Applied Fluid Mechanics at The Johns Hopkins University. His research extends over a wide range of fields, with a common theme involving experimental fluid mechanics and development of advanced optical diagnostics techniques for laboratory and field applications. His group has studied laboratory and oceanic boundary layers; flows in turbomachines; flow-structure interactions; swimming behavior of marine plankton in the laboratory and in the ocean; and cavitation, bubble, and droplet dynamics (the third focusing on interfacial phenomena associated with oil spills). Dr. Katz is a fellow of the American Society of Mechanical Engineers (ASME) and the American Physical Society. He served as editor of the *Journal of Fluids Engineering* and chair of the board of journal editors of ASME. He has coauthored more than 350 journal and conference papers. Dr. Katz was elected to the National Academy of Engineering in 2019. He received a PhD in mechanical engineering from the California Institute of Technology.

Robert P. Lucht is Ralph and Bettye Bailey distinguished professor of combustion in mechanical engineering at Purdue University and director of the Maurice J. Zucrow Laboratories. His present research activities include fundamental experimental and theoretical studies of electronic-resonance-enhanced coherent anti-Stokes Raman scattering (CARS), femtosecond CARS, and polarization spectroscopy, as well as the application of dual-pump CARS and other laser diagnostics for measurements in combustion systems ranging from laboratory flames to gas turbine combustion test rigs. Dr. Lucht has authored or coauthored more than 190 articles in archival journals, and advised or coadvised 40 PhD students. He is a fellow of the Optical Society of America, the American Society of Mechanical Engineers, the American Institute of Aeronautics and Astronautics (AIAA), and the Combustion Institute. In 2008, Dr. Lucht received the AIAA Aerodynamic Measurement Technology Award, and in 2013, he received the Excellence in Research Award from the College of Engineering at Purdue University. He was a participant in a 2019 National Academy study Advanced Technologies for Gas Turbines. Dr. Lucht received a PhD in mechanical engineering from Purdue University.

Hope A. Michelsen is an associate professor in the Department of Mechanical Engineering and in the Environmental Engineering Program at the University of Colorado Boulder. Her research program is focused on developing and using X-ray, optical, mass spectrometric, and theoretical techniques for studying the chemistry and characteristics of combustion-generated particles inside the combustor, and their abundance in the atmosphere. Dr. Michelsen's research experience includes gas-surface scattering experiments, atmospheric modeling, soot-formation studies, combustion-diagnostics development, atmospheric black-carbon measurements, and greenhouse-gas source attribution. She completed a National Science Foundation postdoctoral fellowship at Harvard University in earth and planetary sciences; was a staff scientist at Atmospheric and Environmental Research, Inc.; and was a technical staff member at the Combustion Research Facility at Sandia National Laboratories for 20 years before moving to the University of Colorado. Dr. Michelsen is a fellow of the Optical Society of America and the American Physical Society, a full member of Sigma Xi, an inductee of the Alameda County Women's Hall of Fame, and an associate editor of the *Proceedings of the Combustion Institute*. She received a PhD in chemistry from Stanford University.

Vedha Nayagam is a research associate professor in the Department of Mechanical Engineering at Case Western Reserve University and provides research support to the Microgravity Combustion Branch at the Glenn Research Center of the National Aeronautics and Space Administration (NASA). His areas of research include combustion, fire safety, and fluid physics, with a primary focus on droplet combustion. Dr. Nayagam has more than 25 years of experience in droplet combustion research and has been the principal investigator/project scientist for several NASA-sponsored ground-based and flight (Space Shuttle and International Space Station) experiments involving droplet combustion. Dr. Nayagam has produced more than 50 peer-reviewed journal publications and more than 100 conference presentations. He has received numerous NASA awards, including the Exceptional Public Achievement Medal (2013) for his contributions to droplet combustion phenomena in reduced gravity, and the Silver Achievement Medal (2016) in recognition of cool flame discovery during droplet combustion onboard the International Space Station. Dr. Nayagam is an associate fellow of the American Institute of Aeronautics and Astronautics, a member of the Combustion Institute, and the American Society for Gravitational and Space Research. He received a PhD in mechanical engineering from the University of Kentucky.

Ali S. Rangwala is a professor in fire protection engineering at Worcester Polytechnic Institute. His research interests include problems related to industrial fire and explosion problems. He has worked on such topics as deflagration of combustible dust clouds, ignition behavior of combustible dust layers, in-situ burning of oil, the spread of an oil slick in channels, velocity measuring techniques in fire-induced flows, and flame propagation and burning rate behavior of condensed fuel surfaces. Dr. Rangwala is a recipient of the National Science Foundation Career Award and the Sigma Xi Senior Faculty Research Award. He has published more than 50 journal articles and has presented in more than 60 conferences. Dr. Rangwala received a PhD in combustion and flame spread from the University of California, San Diego.

Abhishek Saha is an assistant professor in the Department of Mechanical and Aerospace Engineering at the University of California, San Diego (UCSD). His research encompasses areas of reactive flows and droplets in connection with power generation, propulsion, and biotransport. Before joining UCSD, Dr. Saha was a member of the research staff at Princeton University. Apart from his research in combustion and multiphase flows, he has served as a reviewer for leading scientific journals and as a panel member in reviewing research proposals submitted to the National Science Foundation. Dr. Saha received a PhD in mechanical engineering and earned the university-wide Outstanding Dissertation Award from the University of Central Florida.

William A. Sirignano, NAE, is Henry Samueli endowed chair in engineering at the University of California, Irvine (UCI). His research interests include spray dynamics and liquid atomization, turbulent combustion and ignition, aerospace propulsion, rocket combustion instability, automotive combustion, fire safety, noise suppression, and applied mathematics. Prior to his time at UCI, Dr. Sirignano served for thirteen years as a faculty member at Princeton University and five years at Carnegie Mellon University. He holds fellow status in the American Institute for Aeronautics and Astronautics (AIAA), the American

Physical Society, the American Society of Mechanical Engineers (ASME), the American Association for the Advancement of Science, the Society for Industrial and Applied Mathematics, and the Combustion Institute. Dr. Sirignano has received numerous awards, including multiple awards from AIAA, the 1996 Alfred C. Egerton Gold Medal from the Combustion Institute, and the 1993 Institute for Dynamics of Explosions and Reactive Systems A.K. Oppenheim Prize. He has served on various boards and committees of the National Academies of Sciences, Engineering, and Medicine, and is currently a member of the National Academies Army Research Laboratory Technical Assessment Board. Dr. Sirignano was elected to the National Academy of Engineering in 2002. He received a PhD in aerospace and mechanical sciences from Princeton University.

Sibendu Som is manager of the Multi-Physics Computation research section in the Energy Systems Division at Argonne National Laboratory and a senior scientist at the Consortium for Advanced Science and Engineering at the University of Chicago. He has more than a decade of experience in enabling technologies for more efficient engine combustion using computational tools. Dr. Som leads a computational fluid dynamics team at Argonne with a research focus on the development of nozzle-flow, spray, and combustion models, using high-performance computing for internal combustion engine applications. His team is responsible for developing predictive simulation capabilities to enable original equipment manufacturers to develop advanced high-efficiency, low-emission engines. Dr. Som has won numerous awards in the field of reacting flows and computational fluid dynamics, together with high-performance computing, including the 2020 Society of Automotive Engineers Fellow Award and the 2020 George Westinghouse Silver Medal. He received a PhD in mechanical engineering from the University of Illinois at Chicago.