PROGRESS REPORT

January 2006 to May 2008

Numerical Simulation of Sour Gas Flares

prepared for:

Air Issues Technical Steering Committee
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ARC Project No.: CEM – 10234-2006
June 17, 2008

Acknowledgements

The authors acknowledge the assistance and guidance from the Air Issues Steering Committee and the project facilitation services of Petroleum Technology Alliance of Canada (PTAC).

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Summary

Hydrogen sulphide (H_2S) is a common component of gas streams flared in Western Canada. Sour gas is flared during well testing, as a means to dispose of sour solution gas, and to provide safe release of sour gas during emergency situations. The impact of H_2S on flare combustion efficiency and overall flare emissions is relatively unknown. Only limited experimental measurements have been reported for flaring of gases containing H_2S, partly due to the hazard and high cost of these type of experiments.

The objective of the project was to develop a numerical simulation tool for a sour gas flare of the type typically used in Alberta. This flare simulation tool would incorporate hydrocarbon and sulphur reaction chemistry in order to predict flare performance for a range of flare operating conditions. The predictions of flame properties and reaction products would give insight into the impact of H_2S and operating conditions on sour flare performance and potential pollutant emissions.

Development of a numerical model and the application of the model to a range of flaring conditions were performed by staff at the Centre for Simulations of Accidental Fires and Explosions at the University of Utah. The numerical flare model used a Large Eddy Simulation (LES) method an incorporated flamelet reaction model for hydrocarbon combustion and sulphur compound reactions. Models for turbulence chemistry interaction were also included.

Development of a reliable and accurate numerical model requires a rigorous program of software development combined with accuracy checking of predictions against experimental data and observations. Initial model simulations were run based on a range of flare conditions from wind tunnel flare tests that were performed previously at the University of Alberta. The LES based model accurately predicted the flame shape and position and also captured the turbulent nature of the flare.

During this project, a reaction model for sulphur species was added to the University of Utah LES model. The model was also modified and methods developed for calculating the predicted combustion efficiency for both hydrocarbons and H_2S. These calculations were based on the time-averaged mass flux of CO_2 and SO_2 leaving the calculation domain.

Work is proceeding to complete a simulation matrix of thirteen flare conditions spanning H_2S concentration from 0 to 30%, wind velocity from 0 to 15 m/s (54 km/h) and flare tip speed from 1 to 15 m/s. These results will be analyzed to better understand the effect of these operating variables on flare performance and sulphur species formed during flaring.

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Numerical Simulation of Sour Gas Flares – Interim Report

1. Background

Sour gas may be flared during well testing, as a means to dispose of sour solution gas or separated acid gases, and for emergency purposes at compressor stations and gas processing plants. Both Alberta and B.C. have ambient air quality guidelines for SO_2 and H_2S that cannot be exceeded during sour gas flaring.

Hydrogen sulphide (H_2S) is a common component of gas streams flared in Western Canada. The impact of H_2S on flare combustion efficiency and overall flare emissions is relatively unknown. The combustion inefficiency of two industrial scale sour gas flares and one sweet gas flare was measured using DIAL equipment in Alberta during 2003 (ARC final report: Well Test Flare Plume Monitoring Phase II: DIAL Testing in Alberta, 2003). The measured mass flux of SO_2 in the flare plume accounted for less than 75% of the H_2S in the flared gas. Further experimental work would be required to determine the other sulphur species that may have been produced during flaring and any impacts that H_2S may have on the combustion of hydrocarbons in a flares. However, experimental work is difficult to perform in wind tunnels due to the safety hazards of H_2S. Testing a range of operating conditions on an industrial sour flare would be difficult and expensive due to H_2S hazards and the height of sour gas flares.

Numerical simulation methods are often used to investigate a wide range of operating conditions when experimentation is difficult or costly. Modern numerical simulation methods have advanced rapidly and are now often used to investigate reacting flow systems, such as coal or natural gas flames, in order to predict pollutant emissions and flame properties. The availability of a simulation tool for sour gas flares that couples hydrocarbon and sulphur chemistry with fluid flow and radiant heat transport will lead to a better understanding of how sour gas flares operate over a range of conditions, sulphur compounds produced during and how these compounds are locally dispersed into the environment. With improved flare source simulations, long-range plume dispersion model predictions may be made more reliable. A numerical model could also be used in future for the design of improved, more effective flares.

2. Objective

The objective of the project was to develop a numerical simulation tool for a sour gas flare of the type typically used in Alberta. This flare simulation tool would incorporate hydrocarbon and sulphur reaction chemistry for prediction of flame shape, temperature and concentrations of both hydrocarbon and H_2S combustion products. The numerical model would be used to predict flare performance for a range of flare operating conditions to give insight into the impact of operating conditions on sour flare performance and potential pollutant emissions from sour flares.

3. Description of Numerical Models Used in this Study

Industrial flares operate under turbulent flow conditions, which involve wide ranges of length and time scales. The biggest of these length scales are in the order of 1 meter and are easily observed with the human eye. The smallest length scales are determined by the fluid viscosity and are in the order of 10^{-10} meters. Time scales range from long, large eddy turnover times, in the order of seconds, to very fast chemical reaction times, in the order of 10^{-9} seconds. In

general, the fuel from the flare tip and ambient air as oxidizer come together in separate streams before mixing takes place. The chemical reactions take place after the fuel and oxidizer is mixed at molecular level. This kind of configuration is referred as non-premixed combustion where the reaction rates are limited by mixing rates.

Detailed chemical mechanisms of combustion reactions involve several thousand elementary reaction steps among hundreds of species with a wide range of time scales. These chemical reactions are exothermic, resulting in both convective and radiative heat transfer. Radiation is the dominant mode of heat transfer at high temperatures, whose transfer depends on the absorptive, emissive, and scattering properties of the gas mixture. The presence of soot in the flame enhances the rate of radiative heat transfer. All of these processes are highly coupled. For example, turbulence enhances mixing and thus chemical reactions. Chemical reaction changes the temperature through the amount of heat generated, and this changes the density and thus the intensity of mixing via turbulence.

Resolving all the length and time scales in practical turbulent combustion applications is not possible even on supercomputers. In general, time-averaged or spatially-filtered governing equations are solved with sub-grid models to represent the unresolved scales and interactions among them. Most commercial fluid simulation codes time-averaging the equations using the Reynolds Averaged Navier-Stokes (RANS) approach. This reduces the computation time but unsteady information such as instantaneous mixing and flame shape can not be captured. Important features of the flame can be captured by resolving large length and time scales responsible for controlling the dynamics, with models for more homogenous smaller scales. This method is called **Large Eddy Simulation** (LES). However, resolving even the large length and time scales requires large amounts of computational resources and requires a massively parallel environment.

3.1 Large Eddy Numerical Simulation Method

Given current modeling options and the importance of unsteady effects that are observed in industrial flares, LES is the prime candidate for modeling such fires. Compared to the traditional Reynolds averaging approach, LES captures the unsteady effects of the flare by explicitly resolving a large portion (theoretically 80%) of the energy containing motions that are responsible for controlling the dynamics of the flare. These large motions are mainly responsible for controlling the air entrainment into the flare and the flare stack-flare fire interaction, two important characteristics that control the shape and stability of the flare. The tradiational RANS methods models all flow scales, and as a result does not capture these important dynamics.

Over the past 10+ years, the Combustion and Reaction Simulations (CRSIM) research group at the University of Utah has been developing a massively-parallel LES code (ARCHES), which is linearly scalable up to 2000 processors, in a component-based framework called Uintah Computational Framework (UCF). The UCF provides the framework for large-scale parallelization of different applications.

LES is employed to model the fluid dynamics and the convection-diffusion scalar transport in the flares. This method successfully captures the transient nature of the coherent vortical structures

responsible for the dynamic features of mixing and flame shape. The LES approach is based on solving the set of density-weighted, filtered, time-dependent, coupled conservation equations for mass, momentum, mixture fraction, and enthalpy in a Cartesian coordinate system as shown below.

$$\frac{\partial \bar{\rho}}{\partial t} + \nabla \bullet (\bar{\rho}\tilde{v}) = 0 \qquad (1)$$

$$\frac{\partial \bar{\rho}\tilde{v}}{\partial t} + \nabla \bullet (\bar{\rho}\tilde{v}\tilde{v}) = -\nabla \bar{p} + \nabla \bullet \bar{\sigma} - \nabla \bullet (\bar{\rho}(\widetilde{vv} - \tilde{v}\tilde{v})) \qquad (2)$$

$$\frac{\partial \bar{\rho}\tilde{Z}}{\partial t} + \nabla \bullet (\bar{\rho}\tilde{v}\tilde{Z}) = \nabla \bullet (\bar{\rho}\tilde{D}_z \nabla \tilde{Z}) - \nabla \bullet (\bar{\rho}(\widetilde{vZ} - \tilde{v}\tilde{Z})) \qquad (3)$$

$$\frac{\partial \bar{\rho}\tilde{h}}{\partial t} + \nabla \bullet (\bar{\rho}\tilde{v}\tilde{h}) = \nabla \bullet (\bar{\rho}\tilde{\Gamma}\nabla \tilde{h}) - \nabla \bullet (\bar{\rho}(\widetilde{vh} - \tilde{v}\tilde{h})) - \nabla \bullet (q_{rad}) \qquad (4)$$

One of the important characteristics of the flaring addressed here is that it occurs in an open domain. Because the open domain must be modeled with a finite numerical domain, pressure-based open domain boundary conditions are employed on all the boundaries except for inlet and crosswind boundary. Boundary conditions for the open domains available in literature proved to be inadequate, so new formulation for the open domain boundary conditions have been developed. At the inlet boundary, the boundary condition is a constant specified mass flux with initially constant velocity profile. At the crosswind boundary, a constant crosswind velocity across the boundary is specified.

In non-premixed combustion, the chemical reactions associated with combustion are fast compared to the sub-grid scale mixing of fuel and oxidizer, thus mixing limits the rate of reactions. Under this assumption and the assumption of equal diffusivity of all species, state space variables such as temperature, density and species concentrations can be expressed as functions of mixture fraction (Z), a conserved scalar. In order to include the effect of enthalpy loss by radiation on the state space variables, an additional parameter, heat loss is also included. Heat loss is a normalized variable describing the amount of sensible enthalpy lost/gained by heat transfer. A non-adiabatic flamelet model is applied to relate the instantaneous state space variables with the mixture fraction and heat loss. In the flamelet model, the chemical reaction is modeled as an opposed-jet diffusion flame and is parameterized using the mixture fraction, heat loss value, and a fixed scalar dissipation rate. At the LES scale, these parameters are tracked on the computational grid and uniquely define the chemical state space for all time and space during the simulation.

Sub-grid scale mixing is modeled by assuming a β-Probability Density Function (PDF) shape in the mixture fraction. Filtered values of the state space variables are computed by convoluting the variables over this prescribed PDF shape. Computing the shape of the β-PDF requires the mean and the variance of the mixture fraction values. Since no transport equation for the sub-grid scale variance is solved, it is modeled using the assumption that the sub-grid scale variance production and dissipation rates are in equilibrium.

ARCHES was developed to address gaseous combustion problems. The presence of the flare pipe in the domain is accounted for by the Material Point Method (MPM). MPM uses material

points (i.e., point masses) to describe the state (i.e., velocities, temperatures, stresses) of the solid. The state of the solid is kept fixed, and so the only effect of MPM, as far as the solid is concerned, is in describing its geometry. The momentum and heat transfer exchange due to the fire-structure interaction are accounted for in the fluid phase, but not in the solid phase. In other words, the temperature rise in the solid pipe is neglected. This is acceptable since the pipe has a high heat capacity, and therefore it would take a long time for the temperature of the pipe to rise significantly. The pipe does, however, radiate heat to the fire, through its specification as a boundary at 298 K. The fire radiates energy to the pipe, and this heat loss is calculated, along with the convective heat transfer implicit in the presence of the wall cell.

3.2 Implementation of Sulphur Reaction Chemistry into the Model

One of the first tasks performed in this project was to select an appropriate sulfur chemistry model to incorporate into the flare simulation model.

A sulfur chemistry model (REI-Leeds sulfur kinetic model) was selected and incorporated into the U. of Utah Large Eddy Simulation model.

3.3 Steps in Performing a Simulation

A typical flare simulation with cross wind takes around two weeks, running the simulation twenty four hours a day to obtain enough computational time to reach a steady-state behavior. Such a simulation requires about 300 processors to run, which translates into about 85K CPU hours (or roughly 9.5 CPU years).

In order to execute any simulation, the chemistry must first be computed and tabulated for use while the simulation is performed. Given a fuel composition, a mixture fraction is defined. Then, various chemical states are determined using the sulphur mechanism for a range of mixture fractions, heat loss values, and mixture fraction variances (for the PDF mixing model). Here, the scalar dissipation value is fixed. Note that there is no need for an ignition mechanism for the code as the chemical state is explicitly defined by the mixture fraction and heat loss values on the grid. Next, the computational domain size is determined depending on the wind characteristics of the particular case. The main objective here is to ensure that the flame is completely enclosed within the computational domain and that the flame front is far away from the boundaries as to limit any boundary condition interaction. The location of the flame front is typically determined by observing profiles of the temperature, or reaction rate of important species (such as CO_2), which are know to be high at the flame front.

During the execution of the simulation, carbon efficiency and sulphur efficiency values are monitored over time. Both these quantities are computed by summing up the outgoing carbon and sulphur leaving the domains in the forms of CO_2 and SO_2 respectively divided by amounts of carbon in the fuel and sulphur in the form of H2S entering the domain through the flare stack. Rolling time averages of the efficiencies are computed using a 1-2 second window. The rolling time average is used as an indication of when steady state is reached, is the rolling average will asymptote to a steady value. After the steady state is reached, the simulation is run to obtain

enough simulated time to collect enough statistics of the carbon and sulphur efficiencies. Figure 1 is an example of how the combustion efficiency, calculated from the mass flux of CO_2 leaving the computation domain varies with time. This fluctuation is a result of the accurate modeling of turbulent flow fluctuations provided by LES modeling.

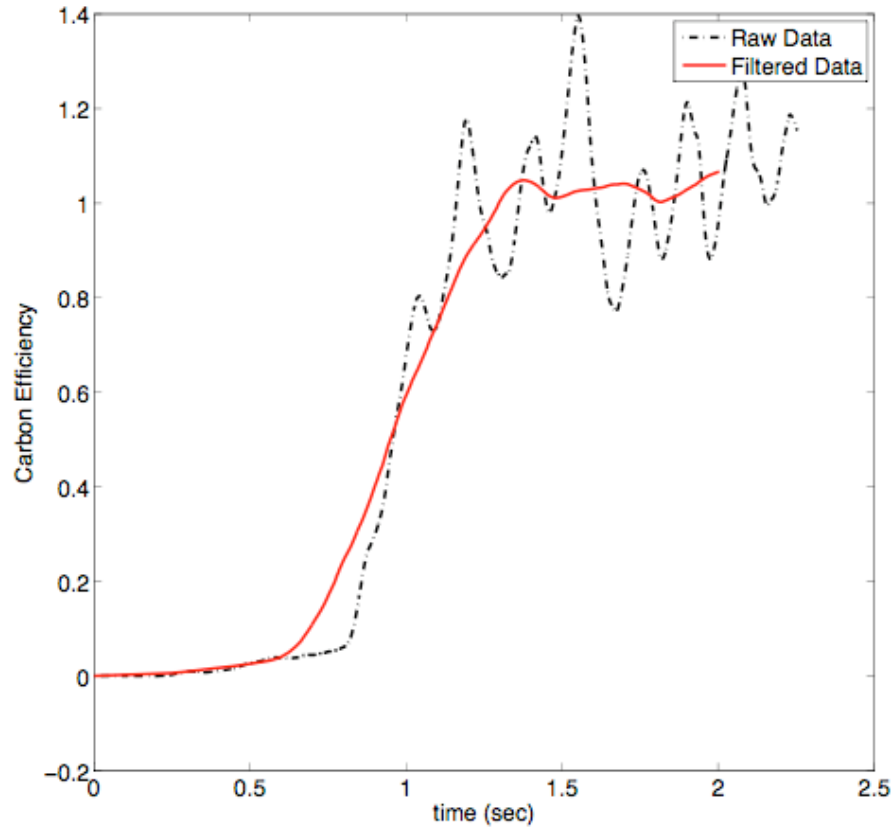


Figure 1: Variation of Predicted Combustion Efficiency with Computation Time

4. Flare Conditions Selected for Simulation

Sour gas flares in Alberta operate under a wide range of conditions. Some of the variables that may affect flare performance include:

- cross wind velocity
- flare tip diameter
- flare tip shielding
- flare gas exit velocity
- heating value of the flared gas
- H_2S concentration.

There are industry design recommendations included in the Alberta Energy Utilities Board Directive 60 Upstream Petroleum Industry Flaring, Venting and Incineration. Directive 60 specifically recommends:

- minimum lower (net) heating value of the flared gas to be 20 MJ/m^3, or as low as 12 MJ/m^3 if the flare stack is designed for local conditions,
- range of stack exit velocities from 1 m/s to 18 m/s, higher velocities up to 122 m/s may be acceptable under certain conditions,
- for non-assisted flares, Log_{10}(maximum exit velocity) = (LHV + 28.8)/31.7, where LHV is the Lower Heating Value of the gas in MJ/m^3 and exit velocity is in m/s.

The formula for calculating maximum exit velocities only limits Vmax to <25 m/s for gas with heating value below 16 MJ/m^3. For a gas with a LHV of 12 MJ/m^3, recommended Vmax is 19 m/s.

Flares of a variety of sizes are used for a large range of operating conditions in the Alberta oil and gas industry. The members of the Air Issues Steering Committee provided a range of operating conditions that can be found for flares operating in Alberta. This range of interest is summarized in Table 1. The upper end of the ranges of exit velocity and H_2S concentration are skewed by emergency flaring cases.

Table 1: Range of Flare Operating Conditions of Interest to Industry

parameter	lower	upper
wind speed (km/h)	0	90
flare tip diameter (cm)	7.6 (3 in.)	46 (18 in.)
flare tip exit velocity (m/s)	1	280
flare gas heating value (MJ/m^3)	12	50
H_2S concentration (%)	0	50

4.1 Base Case Simulation of Well Test Flare

A base case was used for an initial study using the numerical model incorporating sulphur chemistry. The main objective of the base case simulations was to determine grid parameters and domain size for the parametric test simulations. Industrial scale flares require a large domain size to capture important features of the flare, leading to increased numerical solution time and cost. Work with the base case supplied information for selection of solution parameters that would minimize the cost of each simulation without compromising the results.

The base case selected was the well test flare conditions for which Differential Absorption Lidar (DIAL) measurements of hydrocarbons and SO_2 in the flare plume were available (Chambers, 2003). The following summarizes the base case flare:

flare tip:	10.02 inch inner diameter, 10.75 inch outer diameter
fuel gas flow rate:	60,500 Standard m^3/day
tip exit velocity:	13.2 m/s
wind velocity:	2.8 m/s (10 k/s)
gas composition	as in Table 2.

Table 2: Composition of Gas Flow to Sour Well Test Flare

Species	Sour Gas to Flare (%vol)
He	Trace
N_2	0.1718
CO_2	6.1644
H_2S	11.3563
C_1	79.3391
C_2	2.2664
C_3	0.3331
C_4	0.1721
C_5	0.0668
C_6	0.0381
C_7+	0.0918

4.2 Range of Conditions for the Simulation Matrix

A matrix of flaring conditions was developed for the numerical simulations to try to cover the full range of conditions recommended by industry. The length of computing time required to solve each simulation was partly a function of the maximum velocity in the solution domain. Considering the number of cases to run and the computer time available, the maximum flare tip velocity and cross wind speed was limited to 15 m/s (54 km/h) for this study. Some of the parameters were also interrelated. For example, increasing the H_2S content of the flared gas reduces its heating value. Thus conditions such as 50% H_2S content and the maximum heating value of 50 MJ/m^3 would not be a realistic condition.

To reduce the total computing time for the project to a reasonable value, the range of conditions was reduced to a more manageable number of cases by fixing the flare diameter and the gas heating value. The three remaining variables were wind velocity, flare tip exit velocity and H_2S concentration in the flared gas.

To maximize the information on the affect of these three variables from the set of numerical simulations, a Box-Behnken response surface design was used with the remaining three variables:

- wind from 0 to 15 m/s (0 to 54 km/h)
- flare tip exit velocity from 1 to 15 m/s
- H_2S concentration from 0 to 30%

The variables that were held constant in the simulations were:

- flare tip diameter held at 25.4 cm (10 in.),
- hydrocarbons, CO_2, N_2 relative composition in the fuel held the same as the well test flare fuel gas composition,
- atmospheric conditions of 1 atm and 20°C.

The following Table 3 lists the conditions that will be simulated with the numerical model. The total number of simulations using this test matrix design was thirteen conditions.

Table 3: Test Matrix of Parameters to Study Effect of Variables

Test	Wind Velocity (m/s)	Fuel Velocity (m/s)	H_2S content (%)
1	15	15	15
2	15	1	15
3	0	15	15
4	0	1	15
5	15	8	30
6	15	8	0
7	0	8	30
8	0	8	0
9	7.5	15	30
10	7.5	15	0
11	7.5	1	30
12	7.5	1	0
13	7.5	8	15

A separate flare simulation is currently being performed for each of the above conditions. Simulation results for each case will include:

- temperature and gas composition profiles in the flare flame and flare plume immediately downwind of the flame
- mass flow of CO_2 and SO_2 leaving the flare plume
- radiation heat losses from the flame
- relative concentrations of unburnt hydrocarbons and sulphur compounds in the flare plume.

The Box-Behnken experimental design test matrix is an efficient experimental method to maximize the information on effect of variables with a minimum number of experiments. Based on the input variables and measured outputs of the experiments (numerical simulations in this case), a series of quadratic equations will be developed to represent the response surface for the results. These equations will be used to predict combustion efficiency and efficiency of conversion of H_2S to SO_2 over the range of conditions simulated.

5. Numerical Simulation Results

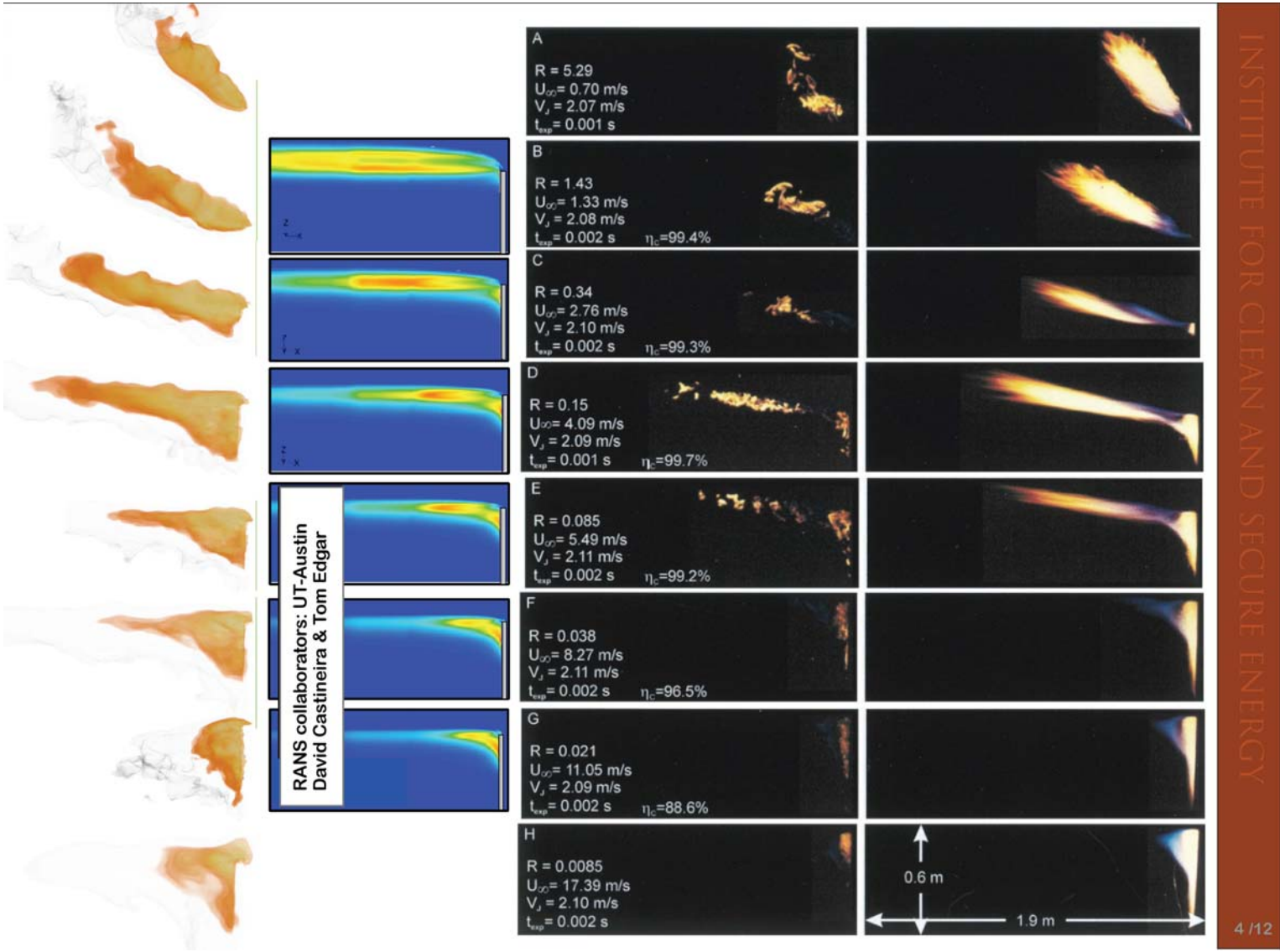
Development of a reliable and accurate numerical model requires a rigorous program of software development combined with checking the accuracy of predictions against experimental data and observations. The experimental data for full scale flares is limited, particularly for sour gas flares. A set of data for a range of conditions for laboratory scale flares without H_2S was available from wind tunnel tests performed at the University of Alberta. The wind tunnel tests included photographs of flame shapes for a wide range of crosswind velocities for a 25 mm diameter flare fired with mixtures of methane, propane and CO_2.

5.1 Predicted Flame Shape

Buoyancy-driven combustion plumes like fires and flares have been particularly difficult to simulate with traditional computational fluid dynamics (CFD) that are based on Reynolds-Averaged Navier-Stokes (RANS) approaches. The large-scale mixing due to vortical coherent structures in these flames are not readily reduced to steady-state CFD calculations with RANS.

Figure 2 compares the numerically predicted flame shape and position with photographs of flares produced in a wind tunnel at the University of Alberta, Edmonton (Kostiuk et al., 2004). The wind tunnel photographs of Figure 2(c) and (d) are for flares with a flare tip diameter of 25 mm and of varying fuel exit momentum and cross wind momentum ratio. The numerical simulations in Figure 2(a) were produced with the LES based model while the simulations in Figure 2(b) were produced with a RANS based model. Figure 2(c) is a short exposure photo of the flame while Figure 2(d) is a long exposure photo that shows the averaged flame shape.

The LES model simulations closely match the shape and position of the wind tunnel flare for the full range of conditions. The turbulent structure of the flame was also predicted with the LES model. This comparison of the LES flare model simulation results with the wind tunnel flare experimental results over a wide range of momentum ratios builds confidence that the LES model is accurately capturing the physical structure of a flare flame.



(a) LES results (b) RANS results (c) wind tunnel flare (d) time-averaged wind tunnel

Figure 2: Visual Comparison of Numerical Simulation and Wind Tunnel Flare Tests

Figure 3 is the predicted flame shape for the base case simulation of the 10 inch diameter well test flare. This flare was operating with a tip velocity of 13.2 m/s and a cross wind velocity of 10 km/s. The simulation result is visually similar to the actual flare.

Figure 3: Predicted Flame Shape for 10 inch Diameter Well Test Flare

5.2 Predicted Reaction Products

Figure 4 is an example result for a simulation with no cross wind. The figure shows predicted temperature profile and SO_2 and SO_3 concentration profiles. SO_2 is present at concentrations up to 3% with maximum concentrations in the regions of highest temperature. SO_3 is present at concentrations of less than 100 ppm, with maximum concentrations in areas outside the zone of high temperature. Thermodynamic equilibrium predicts that combustion of H_2S preferentially forms SO_3 at temperatures below 700ºC while SO_2 is the preferred product above that temperature.

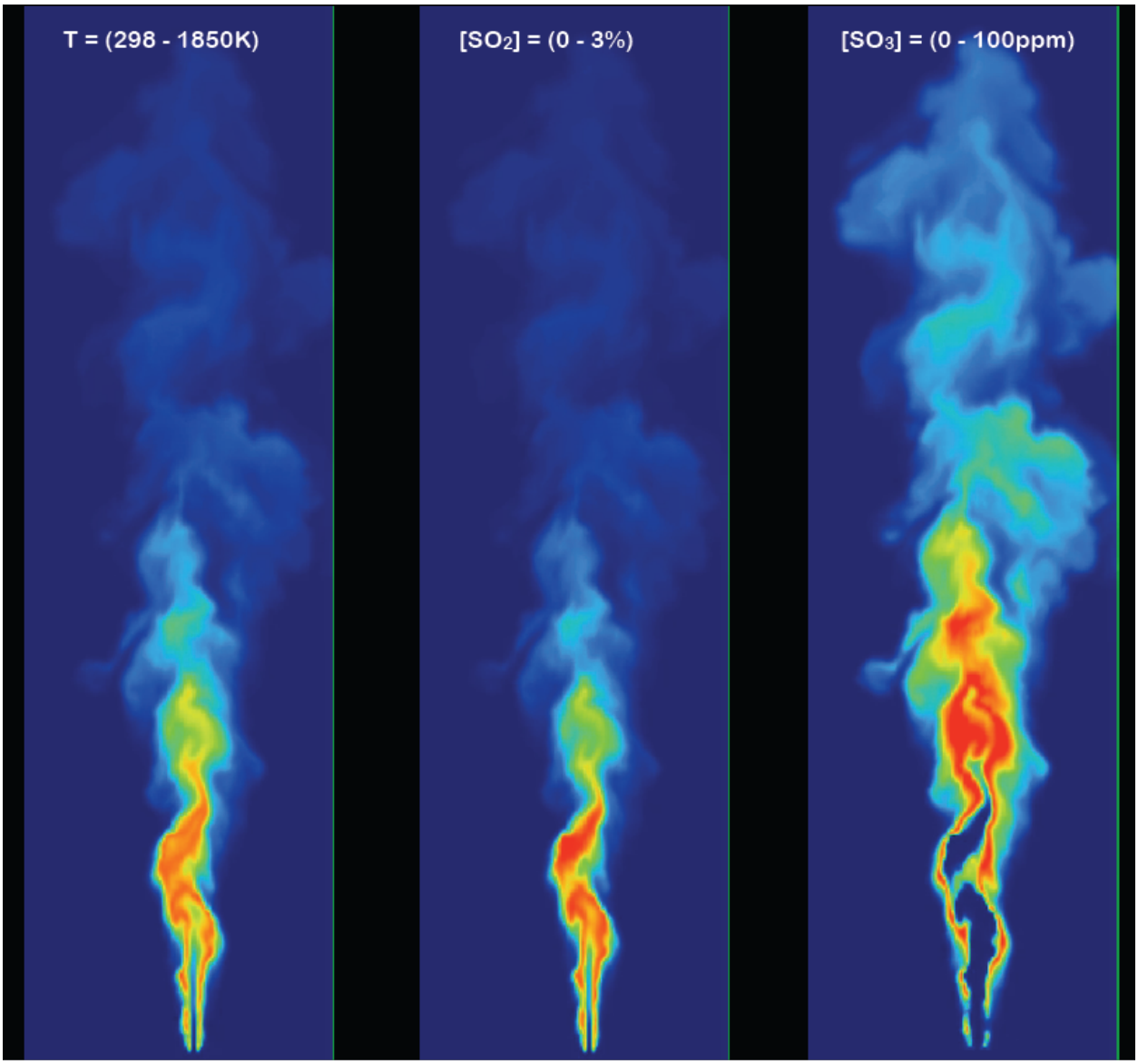


Figure 4: Example Prediction of Temperature, SO_2 and SO_3 Profiles for No Wind Case

6. Next Steps

The remaining cases in the test matrix will be completed and the results analysed. The development of 'empirical' relationships based on the model predictions will be investigated. These simplified relationships would provide a means for industry and/or regulators to estimate a flare's performance and emissions based on operating conditions without the requirement of running the detailed flare simulation tool.

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