CHALLENGES AND PROGRESS IN THE MODELLING OF HEAT TRANSFER AND NO\(_x\) EMISSIONS FROM ROTARY KILN FLAMES INVOLVING UNSTEADY FLOWS

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ABSTRACT

Precessing Jet flames have found significant application in rotary kilns within the minerals processing sector. They typically provide a 5% increase in fuel efficiency and a 40% reduction in thermal NO\(_x\) emissions, caused by increased radiation and, in turn, by increased presence of soot within the flame. The underlying flow-field which generates these flames is very complex, being highly three-dimensional and unsteady. The combination of a highly complex flow, the requirement to model soot and NO\(_x\), combined with Reynolds numbers of 10\(^6\) and kiln lengths of up to 100m, means that the modelling of these flames presents significant challenges to CFD.

A review of recent experimental findings is undertaken to derive an understanding of the underlying mechanisms that control the flames from precessing jet nozzles. This reveals that, although the unsteady near-field flow is necessary to achieve the rapid initial spreading, most of the flame occurs in the downstream region where no true precession occurs. The rapid initial spread causes most of the flame to occur under conditions of reduced global flame strain. This, in turn, promotes soot formation and flame radiation, thereby lowering flame temperature and thermal NO\(_x\) emissions. A review of present models is also undertaken, highlighting strengths and limitations. An analysis of alternative approaches which can be taken to model such flames and the computational requirements and assumptions inherent in each. Finally our progress in modelling is presented along with future directions.

INTRODUCTION

Large-scale unsteady features are present and significant in all turbulent flames and influence the dynamics of their motion (Mungal et al., 1991, Newbold et al., 1997) and entrainment (Muniz and Mungal, 2001). However they are particularly significant in certain classes of flames including the precessing vortex core in swirling flames (Syred and Beer, 1974 and Lucca-Negro and O’Doherty, 2001) and in precessing jet flows and flames (Nathan et al., 1998). The challenge in modelling these unsteady flames at industrial scale is that, in the short to medium term, computational resources will not allow the direct simulation of these three-dimensional, time-dependent features, even before the added complexities of chemical reaction are included. For this reason the development of industrially useful models require the development and evaluation of simplifying approximations, such as those which model the dominant effects of these unsteady turbulent features without simulating them directly. This, in essence, is the approach described by Spalding (1963) as the “art of partial modelling”. The present paper summarises the progress in this approach for the modelling of precessing jet flames.

Precessing jets (PJ) are a class of unsteady flows which have found application in rotary kilns where high radiant heat and low NO\(_x\) emissions are sought. The registered trade name for these burners that utilise the patented (Luxtôn et al., 1988) PJ nozzle is Gyro-Therm®. The precession is generated naturally within a fluidic precessing jet (FPJ) nozzle (Nathan et al., 1998), described later. In gaseous jet flames, the precessing flow results in lower global strain, and so, increased radiant heat transfer and lower thermal NO\(_x\) emissions than simple jet, swirling jet and bluff-body jet flames (Newbold et al., 2000). Pilot scale measurements in a cement kiln simulator have demonstrated that, relative to an optimised high momentum burner, the PJ flow provides about 4% increase in radiant heat-transfer and a shift in the profile toward the burner. It also estimated a reduction in NO\(_x\) emissions, when corrected for differences in heat transfer, of about 30% (Parham et al., 2000). These measurements are consistent with full-scale plant data. In natural-gas-fired cement (Videgar 1997) and lime (Manias et al., 1996) kilns, the precessing jet nozzle is found to typically provide a reduction in specific fuel consumption and/or increase in output by 5 to 10% and a reduction in NO\(_x\) emissions by 30-50%. Similar benefits are found to apply with the combustion of pulverised coal in cement kilns (Nathan and Hill, 2002). However, the combustion
of solid fuels is more complex than that of gas. In addition, the non-uniform distribution of particles, termed “clustering” has been found to be significant in PF flames using PJ nozzles (Smith et al., 2002). For these reasons, the model development to date has focused on gaseous fuels.

The unsteady flow within and emerging from the PJ nozzle is illustrated schematically in Figure 1. The dimensions of the chamber are such that the instantaneous jet attaches asymmetrically within it and emerges from the nozzle at about 45° to the axis (Wong et al., 2002). The asymmetry is accompanied by a rotating pressure field, so that both the internal flow and the emerging jet precess (Nathan et al., 1998). The flow within the chamber is complex, containing large-scale reverse flow zones and a region of swirl at the upstream end of the chamber. The frequency of the precession is two orders of magnitude lower than that of the large-scale motions within the jet itself. This makes modelling using large eddy simulation (LES) computationally prohibitive, since the resolution of both scales of structure requires an extremely large number of time-steps. The modelling of the precession motion within the nozzle using RANS is possible in principle, although its efficacy for application in flames is yet to be adequately assessed. A related large-scale precession motion at a similar Reynolds number has been modelled recently by Guo et al., (2001, 2002) using 3-D, time dependent k-ε model. However the computational resources required for such a simulation are near to the limit of what is achievable with reasonable computing resources. Unfortunately, in the present application the PJ nozzle itself represents less than 1/10,000th of the computational domain of a cement kiln and all of the combustion occurs in the region downstream from it. Hence direct modelling of both the precession motion and the flame at the industrial scale is not realistic for the foreseeable future. To develop simplified approaches, we review the effect of precession on the flow itself and the dominant physical mechanisms by which it influences a flame. We then assess potential modelling approaches and review progress to date.

**Figure 1:** A simplified schematic representation of the flow within the fluidic precessing jet nozzle, as deduced from flow visualisation [Nathan et al., 1998].

### REVIEW OF THE PRECESSING JET FLOW AND FLAME

The precession of the deflected jet which emerges from the nozzle causes the time-mean spreading rate of the jet to be much higher than that of non-precessing jet. However the rate of spread reduces with distance from the nozzle. The effect of the precession on the mixing has been studied by several non-reacting scalar field measurements. Newbold (1997) measured the concentration field, i.e. the mixture fraction, of an unconfined precessing jet flow produced by the fluidic nozzle (Figure 1) in comparison with a simple jet. Parham (2000) studied the effect of a co-flow and confinement on the same flow. Nobes (1997) performed a fundamental study of the effect of precession on the near and far scalar fields of a round jet using a mechanically rotated nozzle to provide well-defined and controllable initial conditions. This nozzle, termed the mechanical precessing jet (MPJ) nozzle is described by Schneider et al. (1997).

A comparison of the scalar measurements of the flows from the FPJ (Figure 2) and MPJ nozzles (Figure 3) shows that, while there are significant differences in the detailed structure, especially in the near field, many of the gross features are similar. Importantly, both jets exhibit a rapid initial spreading followed by the convergence to a far-field flow which is comparable with that of a simple jet. In the near field of the MPJ flow, precession causes the jet to “spiral” into a helix. The precession in this region increases the local strain, causing the helix to rapidly converge upon itself within about 5 nozzle diameters from the exit plane. Figure 3 presents a phase-averaged image of the scalar field from this jet. The laser sheet cuts through the helix, which is evident for approximately one full turn. Downstream from the helix, the jet undergoes a transition to a spreading rate comparable with that of a simple jet. Hence the rapid initial spreading rate does not extend into the far field (Figure 2). Downstream from the transition region, no true precession exists. This is demonstrated by frequency spectra of Schneider (1996) and Mi et al., (1998) which reveal that neither the precession, nor any sub-harmonic, is present beyond about 10 nozzle diameters. This shows that the precession motion does not propagate by vortex pairing, consistent with the flow structure being substantially different from the ring vortices present in a simple jet. In contrast, the near-field flow from the FPJ nozzle does not transcribe a clear helical trajectory (Figure 2). It also has a highly non-uniform initial structure with complex vortex patterns embedded within it (Wong, 2003). Nevertheless, the instantaneous images do not reveal any structure directly associated with precession beyond the near field (Figure 2). Similarly, the frequency of precession is not evident beyond about 5 nozzle diameters.
Figure 2: A comparison of the instantaneous non-reacting mixture fraction of the emerging flows from simple jet (top) and a fluidic precessing jet (bottom) nozzles. The jet initial diameter is 3mm, \( \text{Re} = 20,000 \). [Newbold (1998)].

Although the far field rates of spread and decay are comparable for precessing and simple jet flows, they are not identical. This is consistent with the analytical deduction of George (1989), confirmed experimentally by Mi et al. (2000), that the effect of initial conditions always propagate into the far field. The measurements of Nobes (1997) show that a family of different far-field conditions are produced by varying the Strouhal number of precession (a dimensionless frequency),

\[
St_p = \frac{f_p d_e}{u_e}
\]  

(1)

Figure 3: A comparison of the time-averaged non-reacting mixture fraction from a simple jet nozzle and a precessing jet nozzle. All concentrations are normalised relative to that in the potential core. The jet initial diameter is 3mm, \( \text{Re} = 3,800, \ St = 0 \) (upper) and 0.0063 (lower). [Nobes (1998)].

where \( f_p \) is the frequency of precession, \( d_e \) is the jet exit diameter and \( u_e \) is the exit velocity. The far field rates of spread and decay, and also its virtual origin, are presented for a wide range of, \( St_p \), in Table 1. The values are presented based both on the measurements of half radius and mean centre-line mean values. While some differences are present in the two methods, the broad findings are consistent. It is clear that precession has a dramatic influence on the location of the virtual origin of the far-field, translating it upstream by up to 330 nozzle diameters based on the centre-line decay, and up to 270 diameters based on the half radius. However the far-field rates of spread and decay vary from those of a simple jet by as little as 3% (half radius) and as much as 210% (i.e. just over twice as large). The trends for the F PJ flow are similar with the virtual origin being translated about 100 diameters upstream (Newbold, 1997). This demonstrates that, in a mean sense, precession has a large effect on the location of the virtual origin but a relatively weak effect on the far-field rates of spread and decay.
The four burners of Newbold et al., (2000) were carefully designed to utilise the identical fuel nozzle, (and hence, necessarily to have the same diameter and profile) and the same fuel flow rate. These are shown in Figure 4. The mixing was changed (dramatically) by the use of a co flow of air, for the cases of the swirl and bluff body, and by the use of the PJ nozzle chamber. They found that both the swirling and bluff body flows act to increase global mixing rates and flame strain relative to a simple jet, as evidenced by a reduced flame volume (Figure 4). In contrast, the PJ flame acts to decrease the global mixing rate and flame strain, as evidenced by an increased flame volume (Figure 4). Using an independent measurement of flame strain, also based on the volume rendering technique, Newbold et al. (1999), confirmed that PJ flames have a global flame strain which is an order of magnitude lower than that of a simple jet flame.

Flame strain rate has a dramatic effect on soot formation and flame radiation. This is because, unlike the primary reactions in a flame, the time-scales for the processes of soot formation, growth and oxidation are of the same order as the time-scales of mixing. The pioneering study by Kent and Bastin (1984) shows that the soot volume fraction in a turbulent diffusion flame increases with decreased global strain. The same trend is also found by numerous fundamental studies of laminar flames. At strain rates below the soot-limiting critical strain rate, soot concentration decreases with increasing strain rate (Vandsburger et al., 1984). Decroix and Roberts (2000) also found that the width of the soot field in a laminar counter-flow diffusion flame decreases linearly with the square root of the local strain rate. Recent studies by Qamar et al., (2002, 2003) have confirmed that the reduced strain in the PJ flames results in increased soot volume fraction. It results in three to six times more soot within the base and tip regions of the comparable simple jet flame in unconfined conditions. Those measurements also confirmed the higher soot volume fraction within the PJ flame relative to the swirl and bluff body flames. It is important here to make a distinction between the desirable presence of soot within a flame and the undesirable presence of soot emitted from a flame. Since the soot is consumed within the flame envelope, its presence constitutes neither a loss of combustion efficiency nor an environmental threat.

The presence of soot within a flame acts to increase the flame emissivity. This is because soot produces broad band, incandescent radiation which typically dominates over the narrow-band radiation from inter-molecular processes. Hence flame radiation also scales with the global flame strain. This is demonstrated by the finding of Newbold et al. (2000) that, for all of the four classes of flames with a wide range of different mixing conditions, the radiation from the flame increases with global residence time, or inversely with the global flame strain. This result is shown in Figure 5, where the radiant fraction, $\chi_r$, is defined as the percentage of the total energy of the flame that is released by radiation. That the relationship, perhaps surprisingly, is almost linear, confirms the significance of average flame volume on the radiation. Since the heat losses from a flame are typically dominated by radiation, this implies that the mean flame

<table>
<thead>
<tr>
<th>$St_p$</th>
<th>Exit Angle $\phi$</th>
<th>Decay Rate $D$</th>
<th>Virtual Origin $(x_0/r)$</th>
<th>Half Radius Decay Rate $r$</th>
<th>Half Radius Virtual Origin $r$</th>
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<tbody>
<tr>
<td>0.015</td>
<td>45</td>
<td>0.165</td>
<td>-11.9</td>
<td>0.04</td>
<td>-2</td>
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<tr>
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<tr>
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<tr>
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<tr>
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<td>45</td>
<td>0.078</td>
<td>-332</td>
<td>0.9</td>
<td>-260</td>
</tr>
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</table>

Table 1: A comparison of the far-field rates of spread and decay and virtual origin for precessing jet flows and a simple jet flow [Nobes, 1998]. The simple jet corresponds to the case $St_p = 0$ (i.e. a precession frequency of 0Hz) and $\phi = 0$, (i.e. the initial angle of the jet is equal to that of the nozzle).

When used as gas-fired burner, the PJ flame is typically stabilised a few nozzle diameters from the burner, which corresponds to the end of the near field. Since the flame length is several hundred times the nozzle diameter, nearly all of the combustion occurs within the region where precession is not evident in the cold flow. Various investigations have confirmed that precession is also not evident in most of the flame for the range of Strouhal numbers at which the fluidic PJ nozzle operates. Newbold et al., (1997) analysed the large-scale structures that propagate through the flame using the “volume rendering” technique of Mungal et al. (1991). This is constructed from a time-series of images of the edge of the flame, as determined from the visible light naturally emitted by it. They showed that the frequency of these large-scale motions does not scale with the precession frequency and, indeed, is more than an order of magnitude lower than it. Instead, in an open-flame environment, these large-scale motions are driven by buoyancy, while in a kiln they will be driven by the confined, co-flowing environment. The independence of the large-scale motions within the PJ flame from the precession frequency is further supported by phase-averaged images of the OH radical excited by laser induced fluorescence (Reppel, 2003).

Although there is negligible precession within a PJ flame itself, the effect of precession within the upstream flow produces a dramatic influence on the flame. The rapid initial spreading results in a flame that is typically three times wider than the equivalent simple jet flame with the same fuel and flow rate, although the length of the flame is about the same (Newbold et al., 2000). Furthermore the global characteristics of the flames from the MPJ and FPJ nozzles are similar, provided that the Strouhal number is the same fuel and flow rate, although the length of the flame is about the same (Nathan et al., 1996). The increased width of the PJ flames results in an order of magnitude increase in volume. A global mixing rate can be defined as the flame volume divided by the volume flow-rate of fuel (Turns and Myhr, 1991). On this basis, Newbold et al., (2000) compared the global mixing rate for PJ and simple jet flames along with those of swirl jet and bluff body flames.

The four burners of Newbold et al., (2000) were carefully designed to utilise the identical fuel nozzle, (and hence,
volume has a controlling influence on temperature. Flame radiation controls thermal NOx emissions from simple jet turbulent diffusion flames through its effect on flame temperature (Turns and Myhr, 1991). Newbold et al. (2000) therefore concluded that the global flame strain, through its effect on radiation, has a controlling influence on thermal NOx emissions. The significance of this finding, in the context of modelling, is that the accurate prediction of mean flame volume and strain is of first order importance in predicting flame temperature, and hence, thermal NOx emissions.

In summary, while the precession motion of the jet which emerges from the PJ nozzle is necessary in practice to achieve the rapid initial spreading rates, its effect on the flame is indirect. There is no true precession within most of the flame itself and the dominant mechanism whereby it acts to influence the flame is by reducing the flame strain, so promoting soot formation and radiation. These scale with the mean flame dimensions. Significantly it is also the mean flame shape, flame radiation, flame temperature and thermal NOx emissions that are of greatest interest to designers in prediction of flame performance. On this basis, it can be expected that useful models of the flame may be possible by simulating only the mean flow. This suggests the approach of modelling the rapid initial spreading of the jet computationally, rather than simulating the precession directly.

APPROACHES TO MODELLING THE FLOW

On the basis of the arguments above we have begun developing a two-dimensional, axi-symmetric model of a precessing jet flame in a rotary kiln configuration of relevance to cement and lime production. A detailed description of the approach is provided by Smith et al. (2003a), so only a brief summary is provided here.

The model uses the k-ε formulation because of its robustness and computational efficiency. The transport equation for turbulence energy dissipation, which controls the production and consumption of turbulence kinetic energy, was then modified following previous work by Dally et al., (1998), Morse (1977), Pope (1978) and others to solve the problem of over prediction of the decay rate of a simple jet. This is achieved by making the empirical constants $C_{\epsilon1}$ and $C_{\epsilon2}$, a function of the non-dimensional

$$u_a / u_f = 0.29 \quad u_\Delta / u_f = 0.57 \quad u_\Delta / u_f = 1.71$$

$$u_a / u_f = 0.27 \quad u_\Delta / u_f = 0.54 \quad u_\Delta / u_f = 0.81$$

Figure 4: A comparison of the time-averaged flame shape of flames from a simple jet nozzle (a), a precessing jet nozzle (b) a bluff body nozzle for a range of different air velocities, $u_a$ (c), and for a swirling flame also with different $u_a$ (d). All nozzles have the same central fuel pipe, are fired with propane and have identical fuel velocity, $u_f$, equating to $Re_f = 20,000$ [Newbold et al. (2000)].

Figure 5: The relationship between radiant fraction and global residence time for all of the flames in Figure 4 (Newbold et al, 2000).
axial distance within the near burner region to increase the initial spreading rate caused by the precession. The constants in the far field are set to the values that are standard for a round jet. Using this approach the model avoids the complication of the unsteady motion in the near field while capturing the decay and spreading rates to better predict the flame volume. The classification of the scalar field into two regions, one for the near field and the other for the far field, is justified by the scalar measurements of Parham (2000). Figure 6 shows the near-field and far-field and how the decay rate can be characterised by two rates, separated by an “elbow” point.

The selection of the appropriate constants for the FPJ flow is achieved by calibration against one set of conditions using the scalar measurements of Parham (2000, 2001). These data were obtained for an FPJ flow in a confined co-flowing environment under conditions matching a rotary kiln. The sensitivity of the model to changes in co-flowing environment under conditions matching a rotary kiln is then assessed by comparison with measurements obtained with a different co-flow and confinement is then assessed by comparison with measurements in a 2MW pilot-scale kiln. The combustion model that has been selected is relatively simple because the global strain is low (Newbold et al., 2000). Hence the interaction between the chemistry and the turbulence is negligible and the fast chemistry assumption will be reasonable. This approach, which is usually referred to as “Mixed is Burnt”, decouples the chemical kinetics from the turbulence by using a predetermined PDF distribution (e.g. a Beta function) based on the mixture fraction. This helps minimise the computational expense. Preliminary results using this modelling approach are encouraging.

Figure 6: A superimposition of the instantaneous flow emerging from the FPJ nozzle and the mean centre-line concentration decay determined by planar laser induced fluorescence. Jet Reynolds number = 30,000, working fluid water [Parham (2000)].

Figure 7: A comparison of the computational and experimental time-averaged non-reacting flow from a precessing jet nozzle in a confined co-flowing environment (Smith et al (2003a)).

An alternative simple combustion model which will also be investigated for PJ flames is the Eddy Break-up model, in which the rate of burning is controlled by the rate of turbulent mixing. A generalisation of this model is the Eddy Dissipation Concept which treat reacting eddies as a perfectly stirred reactors. These models allows some finite rate chemistry to be incorporated and are also suitable for simulating soot formation.

The influence of turbulence on soot volume fraction, and hence on radiation, temperature and thermal NOx emissions is anticipated to present a significant challenge to the modelling of PJ flames. Soot modelling has been given a lot of attention over the years, although most investigations have concentrated on diesel engines and gas turbines.

Kennedy (1997) published an excellent review paper on modelling soot formation and oxidation in flames. He classified the models into empirical, semi-empirical and detailed models. Empirical models are usually calibrated using experimental data based on the effective equivalence ratio, C/H ratio and temperature. These models perform relatively well within the environment they were calibrated for but cannot be extended beyond this. The semi-empirical models attempt to incorporate some aspects of the physics and chemistry. Most popular of these is the Magnussen Soot model (Magnussen et al. 1978). This model uses the eddy dissipation concept, with soot being assumed to form in small-scale turbulent structures. The rate of formation of soot nuclei and soot mass is calculated using the model of Tenser et al. (1971). Soot oxidation is assumed to be proportional to the rate of combustion of fuel, ignoring the influences of O2 and OH concentration. The Magnussen model is being used in our calculations since the alternative approaches of detailed modelling of soot are computationally prohibitive for industrial-scale turbulent flames. It is also the standard model used in most CFD packages.

Radiation modelling is also important in PJ flames. A variety of models have been developed to account for radiation heat transfer, each adopting simplifications to make them attractive for industrial applications. The two
main approaches are the Monte Carlo and Discrete Transfer methods. In the former, a photon is selected from a source and tracked through the system until its weight falls below a threshold at which point it “dies”. The photon interaction with its surrounding is then fed back into the energy equation. In this approach a relatively accurate representation of the geometry is required. The second approach, Discrete Transfer Radiation model, can be applied to two dimensional models, such as that of Smith et al (2003). The technique depends on the discretisation of the equation of transfer along rays. Unlike the Monte Carlo simulation the physical quantities of interest are found at fixed points and the zones must be chosen so that the radiation field is reasonably homogeneous inside them. The Rosseland model is one such which can be applied to optically thick media. It uses a simplification of the radiative transport equation by introducing a temperature-dependent diffusion term. The P1 model assumes that radiation intensity is isotropic at a given location in space. For precessing jet flames the optically thin assumption is unlikely to be adequate and the Rosseland model is expected to be appropriate, but with some adjustment to the empirical constants.

Successful prediction of NOx formation in PJ flames is highly dependent on accurate prediction of the temperature (Newbold et al 2000). While the role of soot is expected to be of primary significance, reburn reactions can also be incorporated if necessary. Various models are available for NOx and are usually applied by post-processing due to their negligible influence on enthalpy and strong dependence on temperature.

The incorporation of these models and assessment of their validity is underway using various sources of data. Qamar et al. (2002, 2003) are providing measurements of soot volume fraction in the same open flames for which global measurements of flame volume, radiation and emissions are also available (Newbold et al, 2000). Temperature measurements are also in progress. These measurements can be used in the assessment of the accuracy of soot models in calculating soot volume fraction and its effect on temperature and radiation. The efficacy of the soot models can then be assessed in conditions more representative of an industrial environment using the measurements of Parham et al. (2000). They provide mean flame shape, temperature, radiation, wall temperature, total heat flux and emissions of CO and NOx in a 2 MW cement kiln simulator.

CONCLUSIONS

Precessing jet flows are among those unsteady jet flows with practical significance whose complexity makes them difficult to model. However the review of the mechanisms by which they effect gaseous flames suggests that useful predictions should be possible by modelling the effect of precession on the flow rather than seeking to simulate these effects directly. The review shows that precession acts to rapidly increase the initial spreading rate of the jet. However true precession only occurs in the near-nozzle region, and most of the combustion occurs in the region downstream from this where the flow approaches that of a simple jet. The rapid initial spread causes most of the combustion to occur under conditions of reduced strain relative to a simple jet. This, in turn, causes increased soot volume fraction within the flame, increased radiation, reduced flame temperature and reduced thermal NOx emissions. A two-dimensional RANS model of the non-reacting flow has been developed which reproduces the mean flow with reasonable accuracy. The ongoing program will seek to incorporate models of soot formation which account for the effect of precession on flame strain against emerging in-flame measurements in open flames of both soot volume fraction and flame temperature as well as global performance measurements of Newbold et al., (2000). Model validation will be performed using existing pilot-scale data (Parham et al., 2000).

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