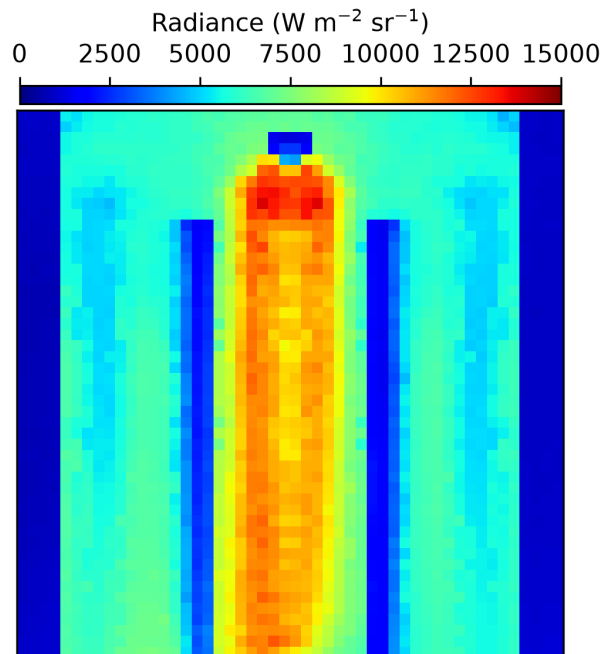




CHALMERS
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Computational Fluid Dynamics Simulations for Infrared Flame-Imaging Analysis

Master's thesis in Applied Mechanics

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Department of Environmental and Energy Sciences

CHALMERS UNIVERSITY OF TECHNOLOGY
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Abstract

Non-intrusive furnace monitoring requires a defensible connection between the radiation recorded by a camera and the combustion state that produced it. This thesis investigates whether changes in the combustion state of a turbulent non-premixed propane–air flame can be distinguished in infrared camera images. Reacting-flow CFD was coupled to spectral ray tracing to connect controlled operating changes, internal temperature and species fields, and the radiance received by a virtual camera.

A steady three-dimensional model of the Chalmers 100 kW unit combined Reynolds-averaged turbulence, finite-rate chemistry with the Eddy-Dissipation Concept, and Discrete Ordinates radiation. The $\lambda = 1.15$ reference was assessed against the 2024 pure-propane measurements before varying excess-air ratio, primary/secondary air distribution, propane flow, and wall condition. CFD temperature and participating-species fields were converted to common-scale 1–5 μm images with a Statistical Narrow-Band Model and ray tracing.

The reference calculation reproduced the measured oxygen-depleted centre and CO-rich core and thereby provided qualitative validation of the principal species topology, although substantial local concentration errors remained. The synthetic images nevertheless distinguished systematic operating changes. Increasing the primary-air fraction moved strong emission towards the burner and shortened the radiating column, whereas secondary-dominant operation produced a longer emitting region. Increasing propane flow strengthened and broadened the column. Changing excess-air ratio altered both its intensity and extent, while a fuel-rich case also demonstrated a cold numerical branch that could not be interpreted as efficient combustion. Imposing a 300 K wall removed most peripheral emission and left a narrower gas-radiation feature, showing that apparent optical flame contraction is not necessarily chemical-flame shortening.

All images use a common 0–15,000 $\text{W m}^{-2} \text{sr}^{-1}$ scale, so their differences reflect the coupled effects of temperature, participating-gas composition, absorption, wall emission, and occlusion. The framework supports qualitative discrimination of simulated flame states, but it is not a calibrated diagnostic for arbitrary camera images. The exploratory machine-learning study is retained in the appendix as a direction for future work.

Keywords: CFD, combustion, propane, infrared imaging, radiation, temperature, species, furnace monitoring.

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List of Acronyms

The acronyms used throughout this thesis are listed below in alphabetical order.

ASCII	American Standard Code for Information Interchange
CAD	Computer-Aided Design
CFD	Computational Fluid Dynamics
DO	Discrete Ordinates
EDC	Eddy-Dissipation Concept
FOV	Field of View
HITEMP	High-Temperature Molecular Spectroscopic Database
IR	Infrared
LPG	Liquefied Petroleum Gas
MAE	Mean Absolute Error
MS	Measurement System
RANS	Reynolds-Averaged Navier–Stokes
RNG	Renormalisation Group
RSM	Reynolds Stress Model
RTE	Radiative Transfer Equation
SNBM	Statistical Narrow-Band Model
SST	Shear-Stress Transport
UDF	User-Defined Function
WSGGM	Weighted-Sum-of-Grey-Gases Model

Nomenclature

The principal symbols, indices, and chemical species used throughout this thesis are listed below.

Latin symbols

A_r	Arrhenius pre-exponential factor for reaction r
$B_\eta(T)$	Spectral black-body intensity at wavenumber η and temperature T
C_i	Molar concentration of species i
$C_{1\varepsilon}, C_{2\varepsilon}, C_\mu$	Constants of the RNG k - ε turbulence model
D_{ij}	Diffusion term in the Reynolds-stress transport equation
e_n	Error between numerical and experimental values at location n
$E_{a,r}$	Activation energy of reaction r
f_p	Fraction of the total air flow supplied through the primary passage
$\text{FOV}_a, \text{FOV}_p$	Azimuthal and polar fields of view
$\mathbf{g}$	Gravitational-acceleration vector
h	Sensible enthalpy
$I(\mathbf{x}, \mathbf{s})$	Radiative intensity at position $\mathbf{x}$ in direction $\mathbf{s}$
$I_b(T)$	Black-body radiative intensity at temperature T
$I_{\eta,j}$	Spectral intensity after traversing layer j
I_{pixel}	Band-integrated intensity assigned to a camera pixel
$\mathbf{J}_i$	Diffusive flux of species i
k	Turbulent kinetic energy
k_{eff}	Effective thermal conductivity
KX	Curtis–Godson accumulated absorption quantity, $\sum_j \kappa_j X_j$
$K\gamma$	Curtis–Godson accumulated pressure-broadening quantity, $\sum_j \kappa_j X_j \gamma_j \delta_j^{-1}$
L_j	Length of ray-path segment j

$\mathbf{m}$	Unit vector defining a camera-ray direction
$\dot{m}$	Mass-flow rate
n_r	Temperature exponent in the Arrhenius expression for reaction r
N	Number of comparison points or terminal ray-layer index, according to context
p	Static pressure
P, P_{ref}, P_s	Gas pressure, reference pressure, and standard pressure
P_k	Production of turbulent kinetic energy
P_{ij}	Production term in the Reynolds-stress transport equation
$\mathbf{q}_r$	Radiative heat-flux vector
R_i	Net chemical production rate of species i
R_{RNG}	Strain-dependent correction term in the RNG k - ε model
R_u	Universal gas constant
r, r_0	Radial coordinate and camera radial position
$\mathbf{s}$	Radiation-propagation direction
S_h	Volumetric source term in the sensible-enthalpy equation
T, T_s, T_w	Gas temperature, standard temperature, and wall or rod temperature
$\mathbf{u}, u'_i$	Mean velocity vector and fluctuating velocity component
$\overline{u'_i u'_j}$	Reynolds-stress component
$\mathbf{x}$	Position vector
x, y, z	Cartesian coordinates
x_c, z_F	Camera-model and Fluent axial coordinates
x_i	Mole fraction of species i
$X_{i,j}$	Optical amount of species i in path segment j
Y_i	Mass fraction of species i
$\dot{\omega}_r$	Kinetic rate of reaction r

Greek symbols

$\alpha_{i,r}$	Reaction order of species i in reaction r
β	Effective broadening parameter in the Malkmus transmissivity relation
γ_i	Pressure-broadening parameter of species i
δ^{-1}	Inverse mean spectral-line spacing
$\Delta\eta_b$	Wavenumber width of spectral band b

ε	Dissipation rate of turbulent kinetic energy
ε_{ij}	Dissipation term in the Reynolds-stress transport equation
ε_w	Wall or rod emissivity
η	Wavenumber
θ	Cylindrical azimuthal coordinate
ϑ, φ	Polar and azimuthal camera-ray angles
κ	Absorption coefficient or band-mean absorption parameter
λ	Excess-air ratio
μ, μ_t	Molecular dynamic viscosity and turbulent viscosity
ρ	Gas density
$\sigma_k, \sigma_\varepsilon$	Turbulent diffusion coefficients in the RNG model
τ	Spectral transmissivity
Φ_{ij}	Pressure–strain redistribution term
ϕ	Generic measured or computed comparison quantity
ω	Specific dissipation rate

Chemical species

C_3H_8	Propane
CO	Carbon monoxide
CO_2	Carbon dioxide
H_2	Hydrogen
H_2O	Water vapour
N_2	Nitrogen
NO	Nitric oxide
NO_x	Nitrogen oxides
O_2	Oxygen
SO_2	Sulfur dioxide

Indices and subscripts

a, p	Azimuthal and polar directions when applied to the field of view
b	Spectral-band index
c	Camera coordinate system
CFD, exp	Computational and experimental values

eff	Effective property
F	Fluent coordinate system
i	Chemical-species or tensor-component index
j	Ray-path segment or tensor-component index
n	Experimental-comparison point index
p, s	Primary-air and secondary-air streams; s also denotes a standard state when attached to P or T
r	Chemical-reaction index
ref, st	Reference and stoichiometric conditions
t	Turbulent property
w	Wall or cooling-rod surface

Measurement labels

M1–M7	Axial measurement stations in the Chalmers combustion unit
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1

Introduction

1.1 Background and motivation

High-temperature industrial processes require stable flames and controlled heat transfer to achieve the desired material temperatures and ensure consistent product quality. Iron-ore pelletization is one such process, requiring furnaces and rotary kilns to operate reliably over extended periods while providing sufficiently high and spatially uniform heat transfer. The transition from fossil fuels to lower-carbon alternatives, such as hydrogen, can alter the composition and temperature of the combustion gases as well as their radiative properties. Therefore, a successful fuel transition must maintain not only the required energy input but also the flame characteristics and heat-transfer conditions necessary for reliable process operation[2, 3]. Monitoring these conditions inside an industrial furnace is difficult. Intrusive probes provide valuable measurements, but only at discrete locations, and their use is limited by high temperatures and harsh operating conditions. Optical measurements offer a non-intrusive alternative. Camera images can capture changes in flame position, size, intensity, shape, and stability, while spectrometric measurements can provide information related to gas temperature and composition [3]. However, an image is not a direct map of the internal combustion state. The intensity recorded by each pixel is the result of radiation emitted and absorbed along a three-dimensional line of sight through the furnace.

Computational Fluid Dynamics (CFD) provides complementary information by resolving the flow, temperature, and species distributions throughout the combustion chamber. In a turbulent non-premixed flame, fuel and oxidizer enter separately, and the reaction zone is governed by their turbulent mixing as well as by chemical kinetics, burner aerodynamics, and heat transfer. Consequently, changes in fuel flow, air distribution, excess-air ratio, or swirl can alter the location and extent of the flame and the associated temperature and species fields [4, 5]. CFD makes it possible to investigate these coupled effects in regions where detailed measurements are difficult to obtain, provided that the numerical model and its limitations are assessed against relevant experimental observations.

Radiative heat transfer provides the physical link between the internal CFD solution and the flame image: the detector records radiation that reaches the camera along its lines of sight. Radiation is a dominant mode of heat transfer in many high-temperature enclosures. In hydrocarbon flames, CO_2 and H_2O emit and absorb radiation in wavelength-dependent spectral bands; the radiation reaching a camera therefore depends on both their concentrations and the temperature distribution

along the optical path [6, 2]. Combining CFD with a spectral radiation model and ray tracing can thus produce synthetic images for which the underlying three-dimensional thermochemical state is known.

Such paired fields and images are useful for developing image-based furnace diagnostics. Experimental images are comparatively easy to acquire, whereas simultaneous measurements of the complete three-dimensional temperature and species fields are generally unavailable. A numerical framework can generate both quantities under controlled operating conditions, thereby providing a traceable basis for studying the relationship between observed radiation and the combustion state.

1.2 Aim

The main aim of this thesis is to determine whether changes in the combustion state of a turbulent non-premixed propane–air flame can be distinguished in infrared camera images. A three-dimensional CFD model is therefore coupled to a Statistical Narrow-Band radiation model and ray tracing to generate synthetic 1–5 μm images for controlled changes in air distribution, excess-air ratio, propane flow, and wall temperature. The images are assessed alongside the calculated temperature and species fields to identify what the observed radiance reveals—and does not reveal—about the underlying flame. Numerical-precision studies support this main aim but are reported separately from the operating-condition study.

1.3 Scope and limitations

The study is limited to steady-state, three-dimensional simulations of a turbulent non-premixed propane–air flame. Conventional air is used as the oxidizer, without additional CO_2 dilution, and the pure-propane condition of Colin et al. [1] is treated as the main experimental reference. The CFD assessment focuses on the available temperature and gas composition measurements and on the principal qualitative structure of the calculated fields. The parametric study considers changes in the excess-air ratio, fuel flow, and distribution of air between the primary and secondary streams.

Within the CFD model, radiative heat transfer is represented using the Discrete Ordinates method together with a Weighted-Sum-of-Grey-Gases Model. The subsequent camera calculation uses the CFD-predicted temperature and the CO_2 and H_2O fields. The selected 1–5 μm spectral range covers part of the infrared spectrum but excludes visible radiation, although the model could be extended to other spectral intervals. The camera is virtual, and the generated images are synthetic radiation images rather than calibrated reproductions of a particular physical sensor. Comparisons are therefore restricted to images created with the same spectral range, radiance scale, camera geometry, orientation, resolution, and cooling-rod configuration.

1.4 Thesis outline

Chapter 2 reviews turbulent non-premixed combustion, CFD modelling, gas radiation, optical diagnostics, and the literature underlying the identified research gap. Chapter 3 presents the furnace geometry, numerical models, validation and model-assessment procedures, parametric simulations, and the spectral-radiation and camera methodology. Chapter 4 reports the CFD and synthetic-imaging results and discusses their relation to the experimental reference. Chapter 5 summarizes the main conclusions and identifies directions for future work.

2

Literature Review

This chapter reviews the literature that underpins the numerical framework developed in this thesis. The discussion first considers the physical mechanisms that govern turbulent non-premixed propane flames and the modelling approaches used to represent them. It then examines radiative heat transfer, optical flame diagnostics, and the use of synthetic images to connect a three-dimensional combustion field to the signal observed by a camera. The chapter concludes by synthesizing these research areas and defining the gap addressed by the present work.

2.1 Turbulent non-premixed combustion

In non-premixed combustion, fuel and oxidizer enter the combustion chamber in separate streams. Reaction can therefore occur only after the streams have mixed at the molecular level. In turbulent flames, this mixing is governed by eddies spanning a broad range of length and time scales, and the location and extent of the reaction zone depend on the interaction between turbulent transport and chemical kinetics. Flame behaviour is consequently sensitive to the fuel and oxidizer flow rates, their momentum ratio, the air-to-fuel ratio, burner geometry, and swirl intensity [4, 7]. Classical treatments of combustion aerodynamics and swirl flows describe how tangential momentum, recirculation, and jet momentum jointly control flame stabilisation and extent [8, 9]. The axial position of a diffusion flame also reflects the balance between buoyancy and inlet momentum [10].

Xi et al. [4] combined experiments and Computational Fluid Dynamics (CFD) to investigate high-pressure turbulent non-premixed swirl flames. They reported that increasing the fuel mass-flow rate produced longer and wider flames, whereas increasing the primary-air-to-fuel mass-flow ratio generally reduced the flame dimensions and moved the flame towards the nozzle. These results demonstrate that global flame dimensions cannot be considered independently of the relative momentum and mixing of the inlet streams.

Swirl provides a further means of controlling mixing and stabilization. Tangential momentum can generate an internal recirculation zone that returns hot combustion products towards the burner, thereby supporting ignition and anchoring the flame. Jarpala et al. [7] found that increasing swirl strengthened the axial reverse-flow region in a non-premixed model gas turbine burner and altered the flame dynamics and pollutant emissions. The effect of swirl is therefore not limited to improved mixing: it also changes residence times and the spatial distributions of temperature and species.

Propane is widely used as a gaseous reference fuel because it permits well-controlled experiments while retaining the characteristic behaviour of hydrocarbon diffusion flames. Abubakar et al. [11] investigated propane–air and propane–oxyfuel flames in a non-premixed, swirl-stabilized combustor. Their results highlighted the role of the interaction between the central fuel jet and the swirling oxidizer in determining flame macrostructure and stability. Altering the oxidizer composition and CO_2 dilution in the oxy-fuel cases also changed the flame shape and anchoring behaviour. In related work, hydrogen enrichment of propane under oxy-combustion conditions modified the stability limits because of the increased fuel reactivity [12]. Although those conditions differ from the air-fired case considered here, the studies show that flame structure cannot be transferred directly between fuels or oxidizer compositions without accounting for changes in chemistry and flow.

Together, these studies identify inlet momentum, swirl, stoichiometry, and fuel composition as coupled controls on a non-premixed flame. This coupling is central to the present study: the Chalmers burner supplies propane and air through separate streams and includes swirling air flows. Changes in its inlet conditions are therefore expected to alter the mixing field and, in turn, the temperature and species distributions used in the radiation calculations.

2.2 CFD modelling of turbulent combustion

Measurements in high-temperature combustion chambers are commonly limited to discrete locations and may be difficult to obtain close to walls, burners, or strong reaction zones. CFD complements these measurements by providing spatially resolved predictions of velocity, turbulence, temperature, species, and heat transfer throughout the domain. Its value is particularly evident in parametric studies, where the response to changes in operating conditions can be investigated without modifying the experimental facility.

The usefulness of a CFD result nevertheless depends on the physical models used to close the governing equations. A turbulent combustion calculation requires models for turbulence, chemical reaction, and turbulence–chemistry interaction, as well as appropriate boundary conditions and a sufficiently resolved representation of the burner. Rajak et al. [5] applied a species-transport formulation to several gaseous fuels, including propane, and demonstrated how such a framework can be used to compare temperature and emission characteristics. Samiran et al. [13] similarly used CFD to study non-premixed LPG combustion with different swirler arrangements, finding that changes in the flow structure affected both temperature and pollutant formation. These studies support the use of CFD for comparative investigations, but their conclusions also emphasize that the predicted combustion field is conditional on the selected numerical formulation.

This model dependence is especially important for swirl-stabilized flames. RANS turbulence models provide an economical description of industrial flows, but different closures may predict the anisotropy, recirculation, and turbulent mixing associated with swirl differently. The resulting changes in residence time and mixture distribution can shift the calculated reaction zone even when the same chemistry model and inlet conditions are used. A turbulence-model assessment against exper-

imental measurements is therefore more informative than selecting a model solely from its performance in a different burner configuration. The standard k - ε framework originates from the eddy-viscosity formulation of Launder and Spalding [14], whereas Reynolds-stress and second-moment closures explicitly address turbulence anisotropy [15, 16, 17].

Errors in one part of a coupled combustion model can also propagate into another. Orbegoso et al. [6] showed that an overprediction of the reaction rate can lead to excessive temperatures and, consequently, an overprediction of radiative heat flux. Agreement in overall flame shape is therefore insufficient when the CFD solution will be used for radiation or camera calculations. The temperature field and the concentrations of the radiatively participating species must also be assessed. For this reason, the present work compares predicted temperature and gas composition with the available measurements before using the CFD fields as inputs to the camera model.

2.3 Experimental reference case

The most directly relevant experimental study is that of Colin et al. [1], who investigated co-firing of gaseous and solid fuels in the Chalmers 100 kW combustion unit. Their campaign covered mixtures from pure propane to pure lignite and included in-flame measurements of temperature and gas composition as well as flame photographs. The pure-propane reference case was operated at approximately 80 kW, with a propane mass-flow rate of 1.73 g s^{-1} and a total air mass-flow rate of 31.01 g s^{-1} at an excess-air ratio of $\lambda = 1.15$.

The reported propane flame was sensitive to its operating conditions. Variations in transport-air flow and excess-air ratio changed its visible appearance, while the measured O_2 and CO profiles indicated a comparatively extended reaction region for the pure-propane case [1]. This sensitivity is consistent with the broader literature on non-premixed swirl flames: redistributing the inlet air changes both the momentum balance and the rate at which fuel and oxidizer mix.

The value of this experiment for the present thesis lies in the combination of complementary observations. Temperature and gas-composition measurements provide quantitative reference data for the CFD model, whereas the photographs describe the externally observable flame. The dataset therefore supports an assessment that extends beyond a comparison of temperature alone and provides the experimental context for linking the internal combustion state to an optical signal.

2.4 Radiation in combustion systems

Thermal radiation is a major mode of heat transfer in furnaces and rotary kilns. Unlike conduction and convection, radiation received at a location depends on the thermo-chemical properties of the medium along the entire optical path. In hydrocarbon combustion products, CO_2 and H_2O are among the principal participating gases. They emit and absorb radiation in discrete spectral bands, so their radiative behaviour is strongly dependent on wavelength, temperature, composition, and path

length [6, 2].

The Radiative Transfer Equation (RTE) expresses the change in spectral intensity along a direction as the combined effect of emission, absorption, and, where relevant, scattering. Within a CFD calculation, solving the RTE together with the flow and energy equations allows radiative exchange between the gas and the enclosure boundaries to influence the predicted temperature field. For a camera calculation, the same physical balance determines the intensity reaching the sensor along each line of sight. The two applications share the same governing physics but impose different requirements on the spectral and directional resolution of the solution.

Detailed line-by-line treatments of gas radiation are computationally costly for three-dimensional industrial CFD. The Weighted-Sum-of-Grey-Gases Model (WSGGM) offers a more economical alternative by representing a non-grey gas as a finite set of grey gases with temperature-dependent weights. Ehlme et al. [2] assessed WSGGM formulations for high-temperature kiln applications involving hydrogen flames and thermal plasmas. They showed that model performance depends on whether the relevant temperature and gas composition fall within the range for which a formulation was developed, and that non-grey effects become particularly important when large gradients occur along a radiative path.

These limitations matter when CFD results are used to predict images. A wall heat-flux calculation may be judged primarily by an integrated energy balance, whereas a camera resolves intensity across many individual rays. Local errors in temperature, CO_2 , H_2O , or spectral absorption can therefore produce spatially structured errors in a synthetic image even when the total heat transfer is reasonable. In the present framework, WSGGM is used in the CFD energy calculation, while a Statistical Narrow-Band Model (SNBM) provides the finer spectral description required in the subsequent camera calculation. Coupled turbulent-combustion and radiation calculations likewise show that radiation can alter the resolved thermal field rather than acting only as a post-processing quantity [18].

2.5 Optical flame diagnostics

Optical diagnostics can observe a flame remotely and thus avoid the flow disturbance, limited spatial coverage, and thermal loading associated with intrusive probes. Conventional photographs and videos provide information about macroscopic quantities such as flame position, projected area, shape, luminosity, and temporal stability. Spectrally resolved measurements provide additional information because the emitted radiation depends on the temperature and composition of the radiating medium. Colin et al. [3] combined spectrometry with monochromatic digital-camera measurements to characterize hydrogen lancing in a pilot-scale rotary-kiln environment. Changes in the injection configuration produced measurable differences in flame area, intensity, shape, and stability, as well as in temperature and NO_x formation. The study demonstrates that optical features respond to changes in the underlying combustion process and can therefore support non-intrusive monitoring during industrial fuel conversion.

An image does not, however, provide a direct two-dimensional map of flame temperature or composition. Each pixel records radiation accumulated along a three-

dimensional line of sight. Radiation emitted by a hot region can be absorbed by intervening gases, which also contribute their own emission before the signal reaches the camera. The relationship between an image and the internal furnace state is consequently non-local and generally non-unique: different distributions of temperature and species may yield similar pixel intensities. Quantitative interpretation therefore requires a forward model that accounts for the geometry and radiative properties of the medium.

2.6 Synthetic radiation imaging

Coupling CFD to a radiative camera model supplies such a forward description. The CFD solution provides three-dimensional temperature and species fields, and ray tracing identifies the sequence of computational cells intersected by each camera line of sight. A spectral radiation model then integrates local emission and absorption along the ray to calculate the intensity at the sensor. Repeating the calculation over the camera field of view produces a synthetic radiation image associated with a known thermo-chemical state.

This approach is also relevant to the longer-term development of data-driven diagnostics. Experiments can provide many flame images, but simultaneous measurements of the complete three-dimensional fields associated with those images are generally unavailable. Numerical modelling can generate paired data: the CFD solution defines the internal state, and the camera model defines its corresponding observable response. Because the operating conditions can be varied systematically, the framework can also be used to examine which changes in the combustion field produce distinguishable image features.

The resulting images must nevertheless be interpreted as model outputs rather than direct substitutes for measurements. Their fidelity is limited by the CFD model, the spectral database and radiation formulation, the representation of the viewing geometry, and any sensor characteristics included in the calculation. Synthetic images are therefore most useful when the assumptions of the complete modelling chain are stated explicitly and its intermediate outputs are assessed against available experimental evidence.

2.7 Industrial context and alternative fuels

The transition from fossil fuels to lower-carbon energy carriers is particularly challenging in high-temperature processes, where a replacement fuel must reproduce not only the required thermal power but also appropriate spatial heat-transfer conditions. Hydrogen combustion, for example, changes both the temperature field and the concentration of radiating species relative to hydrocarbon combustion. These changes affect flame structure, local heat flux, and the optical response of the furnace.

Ehlmé et al. [2] highlighted the importance of suitable gas radiation models when hydrogen flames and other high-temperature heat sources are introduced into kiln environments. Colin et al. [3] showed experimentally that the configuration of hy-

drogen injection influenced flame intensity, area, stability, temperature, and NO_x formation. Taken together, these studies show why energy input alone is an incomplete basis for evaluating industrial fuel conversion.

The propane–air flame considered in this thesis serves as a well-characterized reference case for developing the combined CFD–radiation–imaging method. It does not reproduce the combustion or radiation properties of hydrogen, and conclusions about propane should not be transferred directly to an alternative fuel. It does, however, provide an experimental basis on which the modelling chain can be established before its application to fuels with different thermo-chemical and radiative behaviour.

2.8 Research gap and synthesis

The reviewed literature establishes several components of image-based combustion analysis. Studies of turbulent non-premixed flames demonstrate the sensitivity of flame structure to mixing, inlet momentum, and swirl [4, 7]. Propane experiments show additional effects of oxidizer and fuel composition [11, 12], while the Chalmers experiments provide temperature, species, and image data for the specific pure-propane reference case [1]. CFD studies demonstrate the ability to investigate coupled flow and combustion fields but also expose the dependence of radiation predictions on the combustion solution [5, 6]. Finally, radiation and optical studies establish the physical connection between the internal thermo-chemical state and the externally observed intensity [2, 3].

What remains absent from the literature reviewed here is a general, traceable method that converts three-dimensional CFD fields into spectrally resolved camera images and then relates changes in image structure back to changes in the combustion state. The present thesis develops that forward-modelling method and applies it to the Chalmers propane–air flame. The CFD reference is assessed against the O_2 and CO measurements of Colin et al. [1]; selected operating conditions are then varied before spectral radiative transfer and ray tracing are applied to the resulting temperature, CO_2 , and H_2O fields.

The framework thereby connects three levels of information: the imposed operating conditions, the internal thermo-chemical state predicted by CFD, and the radiation observable by a camera. Establishing and assessing this forward relationship is the focus of the thesis.

3

Methodology

The methodology combined three connected numerical activities: construction of a three-dimensional computer-aided design (CAD) model of the burner and furnace, generation and assessment of a computational mesh, and numerical modelling of the reacting flow and its radiation field. The converged computational fluid dynamics (CFD) solutions were subsequently used as input to a separate virtual infrared-camera model.

The modelling programme was developed in stages. First, the geometry and modelling procedure were checked against the earlier Chalmers oxy-fuel furnace study by Hjærtstam [19]. The fuel was then changed to propane and the principal propane–air operating point was defined from the approximately 80 kW experiment reported by Colin et al. [1]. Alternative turbulence closures and mesh resolutions were compared before the operating parameters were varied. Finally, temperature and participating-gas fields from the CFD solution were post-processed with a statistical narrow-band model (SNBM) and ray tracer to generate line-of-sight infrared intensities.

3.1 CAD model

3.1.1 Furnace and burner representation

The computational geometry was created as a three-dimensional representation of the cylindrical Chalmers furnace and its swirl burner. The furnace section modelled for the camera calculations had an internal radius of 0.400 m and an axial length of 2.400 m. The model included the burner head, the central propane injector, separate primary- and secondary-air passages, the primary and secondary swirl vanes, the furnace chamber, four internal cooling rods, and the lateral exhaust outlet. These features were retained because each influences either the near-burner mixing process, the recirculation pattern, or the line-of-sight radiation received by the camera. The principal furnace dimensions and measurement arrangement were reconstructed from the documented Chalmers facility [20], while the burner passages and swirl geometry were checked against the later detailed burner documentation [21].

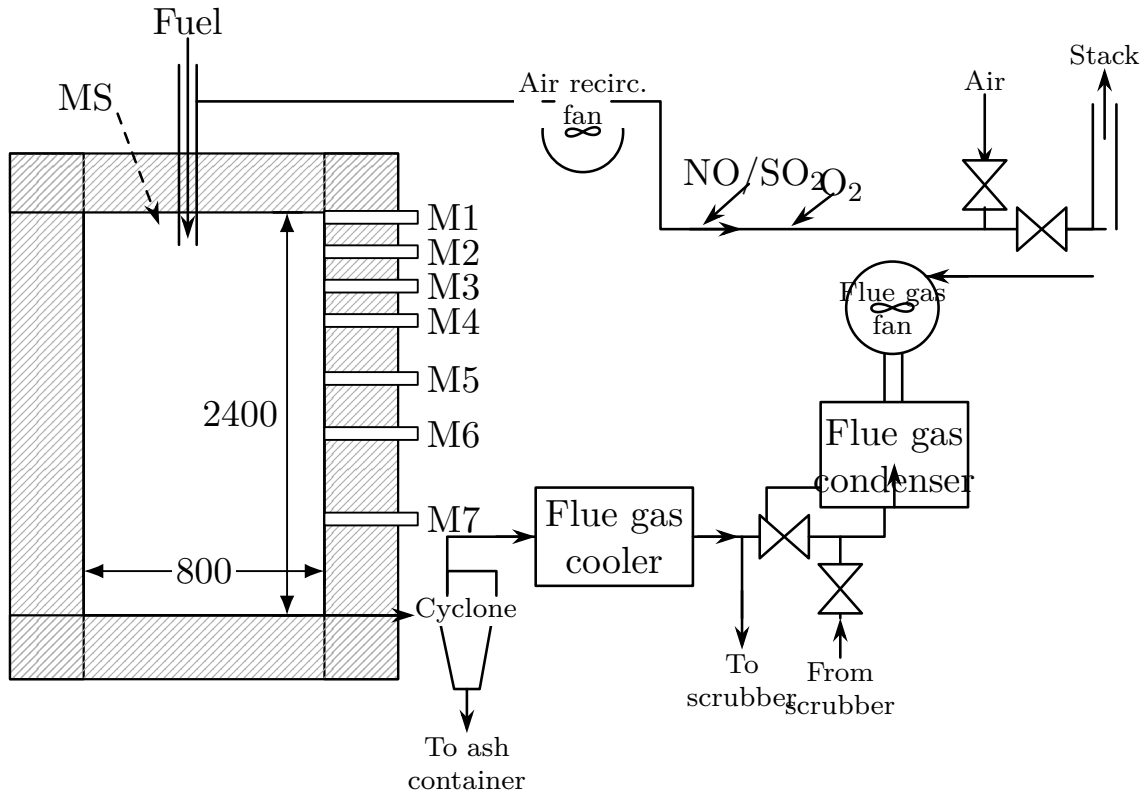


Figure 3.1: Overview of the furnace.

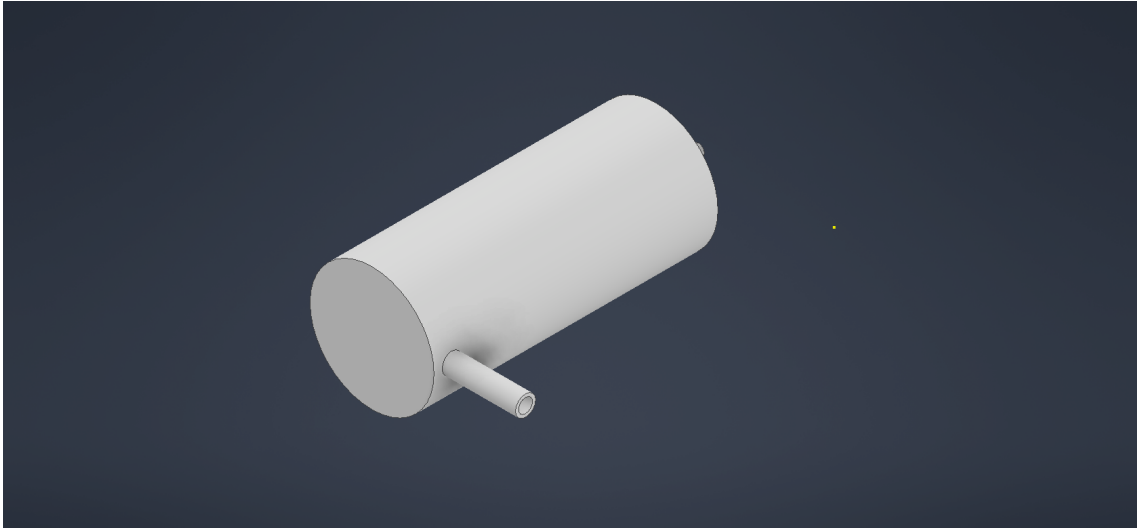


Figure 3.2: CAD representation of the cylindrical furnace chamber and lateral outlet.

3.1.2 Computational boundaries and coordinate systems

The three inlet boundaries were the propane injector, the primary-air annulus, and the secondary-air annulus. The side duct was assigned as the only outlet. All remaining surfaces were walls, with the cooling rods retained as explicit internal

obstacles. This boundary decomposition was used unchanged for both completed turbulence-closure calculations and for the retained RNG $k\text{-}\varepsilon$ case matrix.

The CFD export used the Cartesian coordinates of the Fluent model. In the exported data, the cylindrical furnace occupied approximately $0.4 \leq z_F \leq 2.8$ m. The camera code used a local axial coordinate

$$x_c = z_F - 0.4, \quad (3.1)$$

so that the camera-domain inlet was located at $x_c = 0$ and the outlet end at $x_c = 2.4$ m. The offset in Equation (3.1) was applied only when mapping Fluent data to the camera grid. Camera positions were specified directly in the local coordinate system and were therefore not shifted a second time.

3.2 Meshing

3.2.1 Meshing strategy

The fluid domain was meshed in the watertight-geometry workflow in Ansys Fluent Meshing [22]. A polyhedral volume mesh was selected to represent the complex swirl-vane passages while limiting the number of control volumes in the much larger furnace chamber. Local surface controls were applied to the vane and injector regions, where the strongest velocity and composition gradients were expected. A coarser scale was permitted on the long furnace wall. Ten prism layers were generated on the burner walls, vanes, injector surfaces, furnace walls, and cooling rods to resolve near-wall gradients and provide a gradual transition to the polyhedral core. Table 3.1 lists the recorded controls for the final mesh. The local size assigned to the furnace wall was larger than the global maximum; consequently, it acted as a permissive local control rather than forcing refinement. The global size still limited the volume discretisation in that region.

Table 3.1: Principal settings used for the final computational mesh.

Control or region	Value	Purpose
Global maximum size	15 mm	Furnace volume
Primary and secondary vanes	1 mm	Swirl passages
Injector-hole walls	1 mm	Fuel-jet region
Furnace-wall local control	20 mm	Far-field wall
Local surface growth rate	1.2	Size transition
Prism-layer first height	0.05 mm	Near-wall resolution
Number of prism layers	10	Boundary-layer transition

The resulting final mesh contained 2,096,226 polyhedral cells, 11,144,204 faces, and 8,149,323 nodes in one fluid cell zone. The mesh was generated in millimetres and scaled to metres on import into Fluent. The same final mesh was used for the two

3. Methodology

completed turbulence-model calculations so that changes in the solution could be attributed to the closure rather than to the grid.

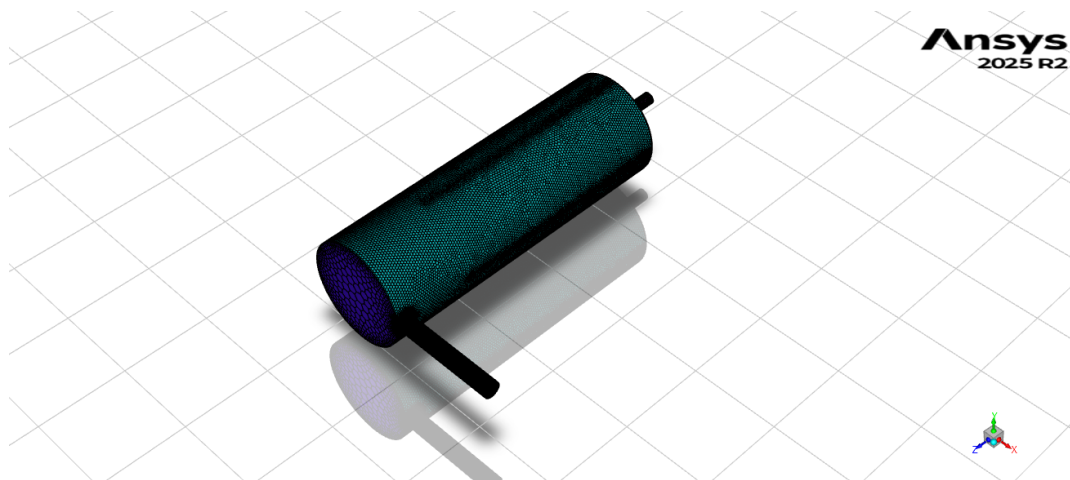
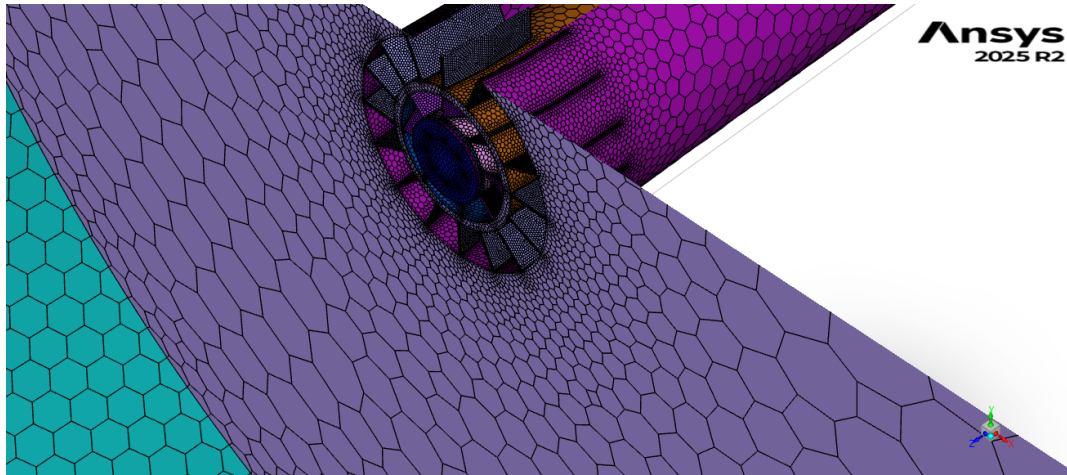
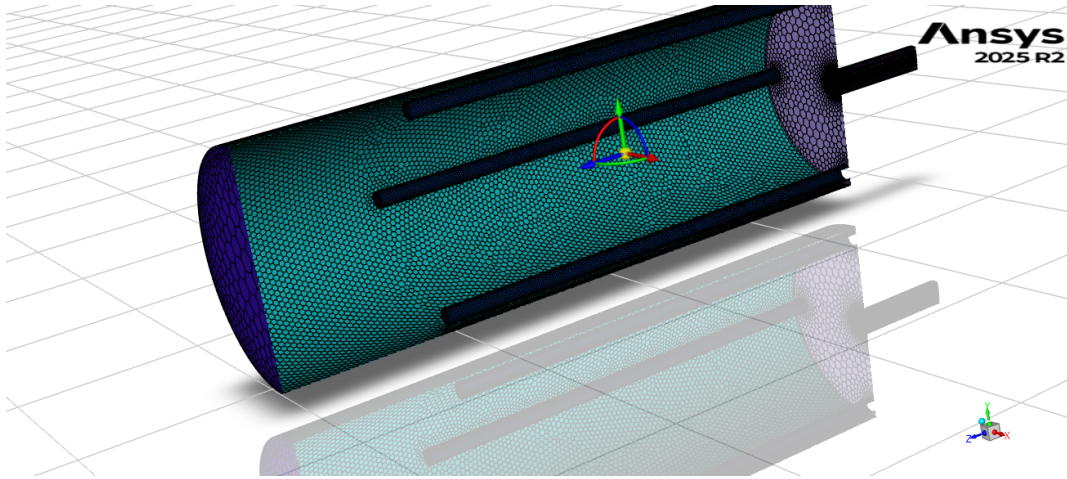


Figure 3.3: Final computational mesh with 2,096,226 polyhedral cells.



(a) Local mesh refinement around the swirl vanes.



(b) Mesh distribution around the cooling rods.

Figure 3.4: Local mesh refinement around the swirl vanes and cooling rods.

The reacting-flow comparison was performed at the reference excess-air ratio of $\lambda = 1.15$. Figure C.1 compares the axial centreline temperature and the radial oxygen and carbon-monoxide profiles at the M2–M5 experimental sampling planes. The three grids contained 769,058, 2,096,226, and 2,930,451 cells. Detailed profile differences and scalar summary quantities are reported in Appendix C. The compact scalar comparison uses the peak centreline temperature and the arithmetic mean of the maximum CO concentration at M2–M5; this definition keeps the summary traceable to the plotted profiles.

The combined mesh-resolution figure and the full numerical comparison are provided in Appendix C.

3.3 Numerical modelling of the reacting flow

3.3.1 Governing equations and numerical framework

The reacting flow was solved in Ansys Fluent using a three-dimensional, steady, pressure-based finite-volume formulation. The gas mixture was treated as a continuum and the Reynolds-averaged conservation equations for mass, momentum, energy, and chemical species were solved. In compact form, continuity and momentum are

$$\nabla \cdot (\rho \mathbf{u}) = 0, \quad (3.2)$$

$$\nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla p + \nabla \cdot \left[\mu \left(\nabla \mathbf{u} + \nabla \mathbf{u}^T \right) - \rho \overline{\mathbf{u}' \mathbf{u}'} \right] + \rho \mathbf{g}. \quad (3.3)$$

The Reynolds-stress term was closed with the turbulence models described in Section 3.3.2. The sensible-enthalpy form of the energy equation can be written as

$$\nabla \cdot (\rho \mathbf{u} h) = \nabla \cdot (k_{\text{eff}} \nabla T) - \nabla \cdot \mathbf{q}_r + S_h, \quad (3.4)$$

where S_h contains chemical heat release and other volumetric energy sources, and $\mathbf{q}_r$ is the radiative heat flux. For species i ,

$$\nabla \cdot (\rho \mathbf{u} Y_i) = -\nabla \cdot \mathbf{J}_i + R_i, \quad (3.5)$$

where Y_i , $\mathbf{J}_i$, and R_i are the mass fraction, diffusive flux, and net chemical production rate, respectively. The formulation follows the Fluent theory documentation [23]. All cases within a comparison set used the same numerical settings and initialisation procedure. Solutions were advanced from a cold-flow or a nearby converged reacting solution. Steady state was assessed from several independent indicators rather than from residuals alone. The scaled continuity, velocity, energy, turbulence, radiation, and transported-species residuals had to decrease and reach a stationary band. Monitored temperatures and species values also had to cease systematic drift. Finally, the boundary fluxes were checked through the mass imbalance

$$\varepsilon_m = 100 \frac{|\dot{m}_{\text{out}} - \dot{m}_{\text{in}}|}{\max(\dot{m}_{\text{out}}, \dot{m}_{\text{in}})} \quad (3.6)$$

and the energy imbalance

$$\varepsilon_E = 100 \frac{|\dot{Q}_{\text{out}} - \dot{Q}_{\text{reaction}}|}{\max(|\dot{Q}_{\text{out}}|, |\dot{Q}_{\text{reaction}}|)}. \quad (3.7)$$

Here, $\dot{Q}_{\text{out}}$ combines the net enthalpy carried through the flow boundaries with heat removed through the walls, and $\dot{Q}_{\text{reaction}}$ is Fluent's domain-integrated heat-of-reaction source. Their signed difference is reported as the net total heat-transfer rate. A quantitative case was required to have stationary monitors and $\varepsilon_E < 5\%$; cases outside this limit were retained only as clearly identified qualitative diagnostics. For the master case ($\lambda = 1.15, 41.15/58.85$), the saved solution at iteration 17,932 had $\dot{m}_{\text{in}} = 0.032739000 \text{ kg s}^{-1}$ and $\dot{m}_{\text{out}} = 0.032738970 \text{ kg s}^{-1}$, corresponding to

$\varepsilon_m = 0.0000913\%$. The heat-of-reaction source was 84.151 kW, the calculated heat output was 85.574 kW, and the resulting net heat-transfer rate and energy error were +1.423 kW and 1.663%, respectively. The final continuity and energy residuals were 8.05×10^{-4} and 3.70×10^{-5} ; the saved residual histories were stationary over their final iterations. The master case therefore satisfied the adopted steady-state checks. The same flux calculation for the full parametric matrix is documented in Appendix D.1.

3.3.2 Turbulence closures

Two Reynolds-averaged turbulence closures were compared on the final mesh because the burner contains strong streamline curvature, vane-generated swirl, and recirculation. Bäckström and Jilvero recommended the Reynolds stress model (RSM) for earlier CFD calculations on the Chalmers unit [24]. The RSM was therefore considered during model planning, but no complete, directly comparable RSM result was available for the present propane–air case matrix. It is not presented as an assessed closure here.

3.3.2.1 RNG k - ε

The renormalisation-group (RNG) k - ε model solves transport equations for turbulent kinetic energy k and its dissipation rate ε :

$$\nabla \cdot (\rho \mathbf{u} k) = \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \nabla k \right] + P_k - \rho \varepsilon, \quad (3.8)$$

$$\nabla \cdot (\rho \mathbf{u} \varepsilon) = \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \nabla \varepsilon \right] + C_{1\varepsilon} \frac{\varepsilon}{k} P_k - C_{2\varepsilon} \rho \frac{\varepsilon^2}{k} - R_{\text{RNG}}, \quad (3.9)$$

$$\mu_t = \rho C_\mu \frac{k^2}{\varepsilon}. \quad (3.10)$$

The additional RNG strain-dependent term R_{RNG} modifies the dissipation response in rapidly strained flow [25]; its Fluent implementation is further documented in the turbulence theory guide [26]. The RNG model provided the main engineering closure for the final parametric study.

3.3.2.2 SST k - ω

The shear-stress-transport (SST) model blends a k - ω formulation near solid surfaces with a transformed k - ε behaviour away from the wall. Its eddy viscosity is limited by the turbulent shear stress, which improves its response to adverse pressure gradients and separation [27]. It was included to test the sensitivity of the near-burner recirculation and flame anchoring to the wall treatment and eddy-viscosity closure. Chemistry, radiation, mesh, and boundary conditions were held fixed in the completed RNG k - ε /SST k - ω comparison. The RNG k - ε solution was retained for the operating-condition matrix because it provided the most robust common basis for completing that matrix. This choice does not contradict the earlier RSM recommendation, which concerned a different fuel and modelling objective.

3.3.3 Species transport and turbulence–chemistry interaction

The gaseous combustion process was represented using species transport with a finite-rate mechanism and the eddy-dissipation concept (EDC). The transported species were C_3H_8 , O_2 , N_2 , CO_2 , CO , H_2O , and H_2 . Nitrogen acted as the inert balance species. EDC embeds finite-rate reactions in turbulence-controlled fine structures and was used to couple the Jones–Lindstedt chemistry to the RANS turbulence field. The volumetric finite-rate formulation follows the Fluent reacting-flow theory documentation [28].

The global propane mechanism was based on Jones and Lindstedt [29]. In the user-defined function (UDF), reversible water–hydrogen and water–gas-shift steps were entered as separate forward and reverse reactions, giving the six irreversible rate expressions in Table 3.2.

Table 3.2: Global reactions implemented in the Jones–Lindstedt UDF.

No.	Reaction	Rate dependence
1	$\text{C}_3\text{H}_8 + 1.5\text{O}_2 \rightarrow 3\text{CO} + 4\text{H}_2$	$[\text{C}_3\text{H}_8]^{0.5}[\text{O}_2]^{1.25}$
2	$\text{C}_3\text{H}_8 + 3\text{H}_2\text{O} \rightarrow 3\text{CO} + 7\text{H}_2$	$[\text{C}_3\text{H}_8][\text{H}_2\text{O}]$
3	$\text{H}_2 + 0.5\text{O}_2 \rightarrow \text{H}_2\text{O}$	$[\text{H}_2]^{0.25}[\text{O}_2]^{1.5}$
4	$\text{H}_2\text{O} \rightarrow \text{H}_2 + 0.5\text{O}_2$	$[\text{H}_2]^{-0.75}[\text{O}_2][\text{H}_2\text{O}]$
5	$\text{CO} + \text{H}_2\text{O} \rightarrow \text{CO}_2 + \text{H}_2$	$[\text{CO}][\text{H}_2\text{O}]$
6	$\text{CO}_2 + \text{H}_2 \rightarrow \text{CO} + \text{H}_2\text{O}$	$[\text{CO}_2][\text{H}_2]$

For reaction r , the kinetic rate had the Arrhenius form

$$\dot{\omega}_r = A_r T^{n_r} \exp\left(-\frac{E_{a,r}}{R_u T}\right) \prod_i C_i^{\alpha_{i,r}}, \quad (3.11)$$

where the concentration C_i was expressed in kmol m^{-3} . Table 3.3 gives the constants implemented in the UDF.

Table 3.3: Arrhenius constants used in the six UDF reaction-rate expressions.

No.	A_r	n_r	$E_{a,r}$ (J kmol^{-1})
1	4.00×10^{11}	0	1.2552×10^8
2	3.00×10^8	0	1.2552×10^8
3	8.50×10^{15}	−1	1.6736×10^8
4	2.52×10^{19}	−1.5	4.1490×10^8
5	2.75×10^9	0	8.3680×10^7
6	9.268×10^{10}	0	1.1760×10^8

Several safeguards were included to make the compiled rate routine robust during initialisation and EDC iteration. Arrhenius temperatures were limited to 300–2500 K, non-positive concentrations returned zero for positive reaction orders, and a concentration floor of $10^{-4} \text{ kmol m}^{-3}$ was used for the negative hydrogen order in reaction 4. The returned rate was bounded between zero and $10^6 \text{ kmol m}^{-3} \text{ s}^{-1}$. These limits prevent floating-point overflow and singular behaviour at vanishing hydrogen

concentration; they are numerical implementation bounds rather than additional chemical reactions.

3.3.4 Radiation model in CFD

Radiative heat transfer in the CFD model was calculated using the discrete ordinates (DO) method [30]. For direction $\mathbf{s}$, the radiative transfer equation for an emitting-absorbing gas is

$$\mathbf{s} \cdot \nabla I(\mathbf{x}, \mathbf{s}) = \kappa [I_b(T) - I(\mathbf{x}, \mathbf{s})], \quad (3.12)$$

with the same angular discretisation retained across the comparative cases. The weighted-sum-of-grey-gases model (WSGGM) supplied gas emissivity as a function of temperature and the CO_2 – H_2O composition. The Fluent implementation is based on Smith et al. [31, 2]. This CFD radiation solution affected the gas energy balance and the predicted wall heat transfer. It is distinct from the narrow-band camera post-processing described in Section 3.4: WSGGM was used inside the CFD calculation, whereas SNBM was used to resolve the spectral intensity observed by the virtual camera.

3.3.5 Boundary and operating conditions

The baseline propane–air condition followed Colin et al. [1]. Pure propane entered through the central injector at a mass flow rate of 1.73 g s^{-1} and a total temperature of 300 K. The combined air flow was 31.01 g s^{-1} , corresponding to an excess-air ratio $\lambda = 1.15$. Primary and secondary air entered at 300 K with an oxygen mole fraction of 0.21 and nitrogen as the balance. The baseline split was 41.15% primary air and 58.85% secondary air, giving 12.761 and 18.248 g s^{-1} , respectively. The lateral exhaust was represented by a pressure outlet. Solid boundaries were no-slip walls and the cooling rods were treated as impermeable wall surfaces.

The inlet conditions were taken from Colin et al., but they were applied to the reconstructed Chalmers geometry used in this thesis, including its cooling rods. The calculation is therefore an assessment against the published propane–air measurements, not an exact numerical reproduction of the experimental configuration.

Table 3.4: Principal boundary conditions for the baseline propane–air case.

Boundary	Type	Mass flow	Boundary data
Propane injector	Mass-flow inlet	1.730 g s^{-1}	300 K, pure C_3H_8
Primary air	Mass-flow inlet	12.761 g s^{-1}	300 K, $x_{\text{O}_2} = 0.21$
Secondary air	Mass-flow inlet	18.248 g s^{-1}	300 K, $x_{\text{O}_2} = 0.21$
Side exhaust	Pressure outlet	Solution dependent	Prescribed pressure
Walls and rods	No-slip wall	0	Radiation coupled

An additional case prescribed a uniform wall temperature of 300 K to test the sensitivity of the reacting flow and camera input fields to the wall thermal condition. It was treated as a sensitivity case and not as a replacement for the principal boundary-condition set.

Comparisons with the experiment used paired quantities at matching axial and radial locations wherever the measurement coordinates were available. The assessment included local profiles and two-dimensional contours, since an acceptable mean value can otherwise conceal an incorrect flame length, recirculation zone, or radial gradient.

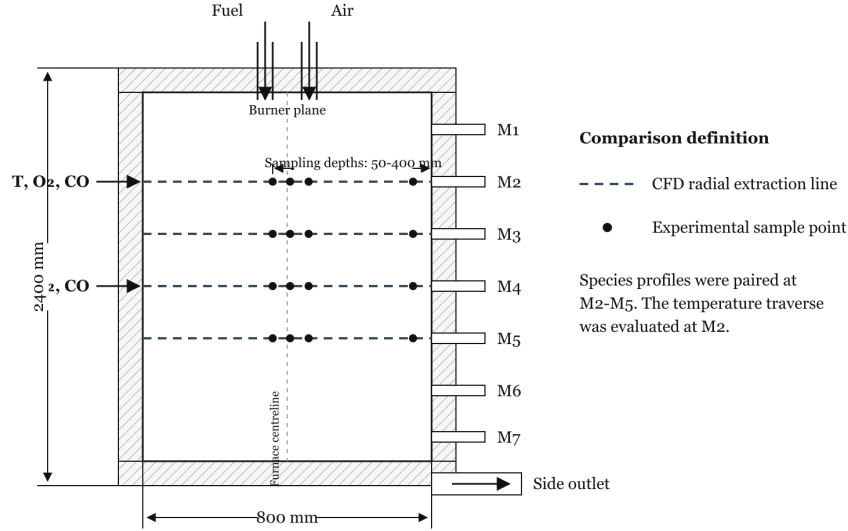


Figure 3.5: Experimental sampling locations and corresponding numerical extraction lines used for temperature, O_2 , and CO comparisons.

3.3.6 Parametric case matrix

The excess-air ratio was defined as

$$\lambda = \frac{(\dot{m}_{\text{air}}/\dot{m}_{\text{fuel}})}{(\dot{m}_{\text{air}}/\dot{m}_{\text{fuel}})_{\text{st}}}. \quad (3.13)$$

At a fixed propane flow of 1.73 g s^{-1} , four values of λ were simulated. The corresponding combined air flows are listed in Table 3.5.

Table 3.5: Excess-air-ratio cases at $\dot{m}_{\text{C}_3\text{H}_8} = 1.73 \text{ g s}^{-1}$.

λ	Total air flow (g s^{-1})	Mixture description
0.600	16.20	Fuel rich
1.000	27.00	Stoichiometric
1.150	31.01	Reference excess air
1.623	43.76	High excess air

For each excess-air condition, the combined air flow was divided between the primary and secondary passages using primary/secondary percentages of 10/90, 25/75, 41.15/58.85, 58.85/41.15, 75/25, and 90/10. If f_p is the primary fraction, the inlet flows were calculated from

$$\dot{m}_p = f_p \dot{m}_{\text{air}}, \quad \dot{m}_s = (1 - f_p) \dot{m}_{\text{air}}. \quad (3.14)$$

This matrix separated the effect of global mixture strength from redistribution of the same total oxidiser flow between the two swirl passages.

A second series varied the propane flow while retaining $\lambda = 1.15$ and the reference 41.15/58.85 air split. The prescribed flows are shown in Table 3.6.

Table 3.6: Fuel-flow series at $\lambda = 1.15$ and the reference air split.

Propane (g s ⁻¹)	Total air (g s ⁻¹)	Primary air (g s ⁻¹)	Secondary air (g s ⁻¹)
1.00	18.02	7.416	10.604
1.50	27.03	11.123	15.907
2.00	36.04	14.831	21.209
3.00	54.06	22.247	31.813

3.3.7 Field export for radiation post-processing

Converged solutions were exported as Fluent ASCII data. The volumetric file contained Cartesian coordinates, temperature, and the CO₂ and H₂O mole fractions. Variables were selected by header name during post-processing rather than by column position; this prevented the species columns from being interchanged when the export order changed. The final fluid export contained approximately 2.1 million rows, of which approximately 1.05 million points lay inside the cylindrical camera domain. The maximum nearest-grid mapping distance was approximately 0.011 m and the exported peak temperature was approximately 2250 K.

Wall data were exported separately. Side-wall and end-disc points were identified and interpolated independently to avoid applying a cylindrical-wall mapping to the furnace ends. The final coordinate interpretation for the wall file was (z, x, y) , which reduced the mean nearest-wall interpolation distance to approximately 0.021 m. Cooling-rod surfaces were represented separately by the documented geometry described in Section 3.4.4.

3.4 Numerical modelling of the virtual infrared camera

3.4.1 Purpose and modelling assumptions

The camera model converted a three-dimensional CFD solution into a two-dimensional map of band-integrated radiative intensity. It represented an idealised, uncalibrated

infrared imager rather than a specific commercial sensor. The model included emission and absorption by H_2O and CO_2 , emission from the furnace wall and cooling rods, and geometrical occlusion. Soot, particles, and scattering were disabled in the present calculations. Wall reflection and incident reflected radiation were also set to zero; the surface source therefore comprised emitted radiation only. The present work was limited to the infrared part of the spectrum. The general radiative-transfer framework can also be applied in the visible range when suitable spectral properties and detector limits are supplied, but that route was outside the scope of this study. The main implemented spectral window was $1\text{--}5\ \mu\text{m}$, equivalent to $2000\text{--}10000\ \text{cm}^{-1}$. The spectral limits were parameters rather than an assumed detector specification, so alternative windows could be used for sensitivity studies without changing the ray geometry.

3.4.2 Interpolation to the cylindrical camera grid

After applying Equation (3.1), each Fluent point was converted to cylindrical coordinates,

$$r = \sqrt{x^2 + y^2}, \quad \theta = \text{atan2}(y, x), \quad (3.15)$$

with negative angles wrapped to $0 \leq \theta < 2\pi$. Explicit wrapping was required to prevent half of the furnace from being placed in the first angular sector. Temperature and mole fractions were mapped to the regular cylindrical grid using nearest-neighbour lookup with a k -d tree. A uniform offset of 0.001 was added to both participating-gas mole fractions in the implemented pre-processing routine as a numerical safeguard for the spectral calculation.

The baseline post-processing grid contained 10 radial, 32 circumferential, and 50 axial cells; this optional resolution was selected to limit the time and memory required for image generation. A refined grid with $20 \times 64 \times 100$ cells was used to assess post-processing resolution. This refinement was important because the cooling rods subtended only about 9° , so the 32-sector grid could under-resolve their angular extent.

3.4.3 Camera geometry and ray generation

The camera centre was placed 5 mm inside the furnace wall at $r_0 = 0.395\ \text{m}$, $x_{c,0} = 0.415\ \text{m}$, and a model azimuth of $\theta_0 = 45^\circ$. Its optical axis was directed towards the furnace centreline. The standard synthetic image contained 50×50 pixels. The wide-view configuration used azimuthal and polar fields of view of 123.5° and 103.5° , respectively. A narrower $35^\circ \times 29.3^\circ$ configuration was additionally available for a rod-free central view.

One ray was traced for each pixel. Before rotation to θ_0 , directions were sampled

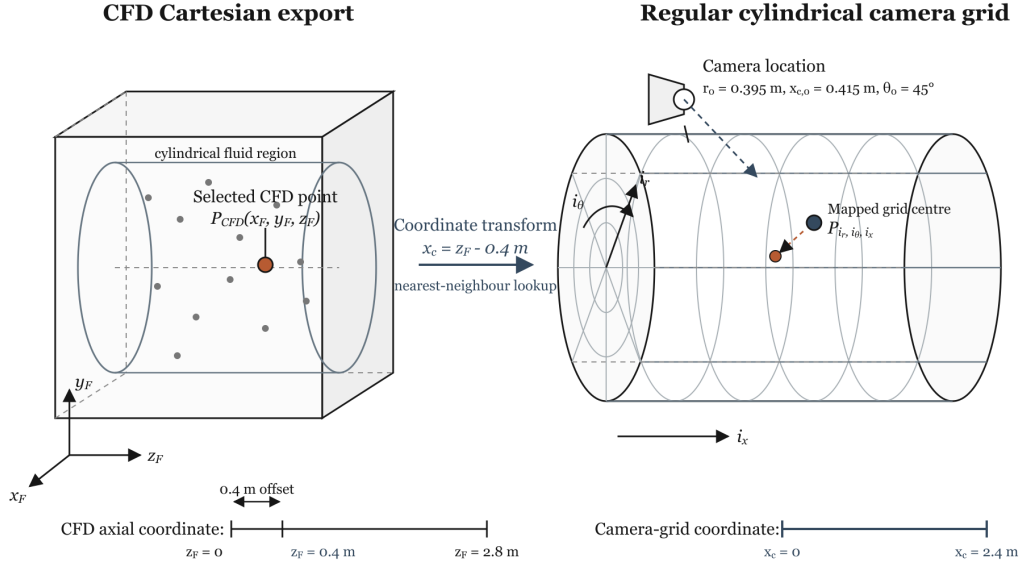


Figure 3.6: Transformation and nearest-neighbour mapping from the Cartesian CFD export to the regular cylindrical camera grid. The local axial coordinate is obtained from $x_c = z_F - 0.4$ m.

from a spherical fan centred at 90° :

$$\vartheta \in \left[90^\circ - \frac{\text{FOV}_p}{2}, 90^\circ + \frac{\text{FOV}_p}{2} \right], \quad (3.16)$$

$$\varphi \in \left[90^\circ - \frac{\text{FOV}_a}{2}, 90^\circ + \frac{\text{FOV}_a}{2} \right], \quad (3.17)$$

$$\mathbf{m} = (\sin \vartheta \cos \varphi, \sin \vartheta \sin \varphi, \cos \vartheta). \quad (3.18)$$

The resulting direction was rotated about the furnace axis so that the central pixel intersected the centreline. This construction preserved the same geometrical definition when the camera azimuth or field of view was changed.

3.4.4 Ray marching and surface treatment

Each ray was advanced in 0.01 m increments through the cylindrical grid, with a maximum of 1000 steps. Radial, angular, and axial indices were calculated from the ray location, and path length was accumulated when a ray entered a new cell. Integration extended from the camera to the first solid boundary visible along that line of sight. The stored path was then traversed in reverse for the radiative-transfer calculation.

The four cooling rods were represented by their documented cylindrical geometry: approximately 0.060 m diameter, 0.351 m pitch radius, azimuths of 0° , 90° , 180° , and 270° , and an axial extent of $0 \leq x_c \leq 1.79$ m. They were treated consistently as opaque solid surfaces in all reported images. Where a line of sight intersected a rod, the rod surface supplied the boundary emission before gas absorption and emission

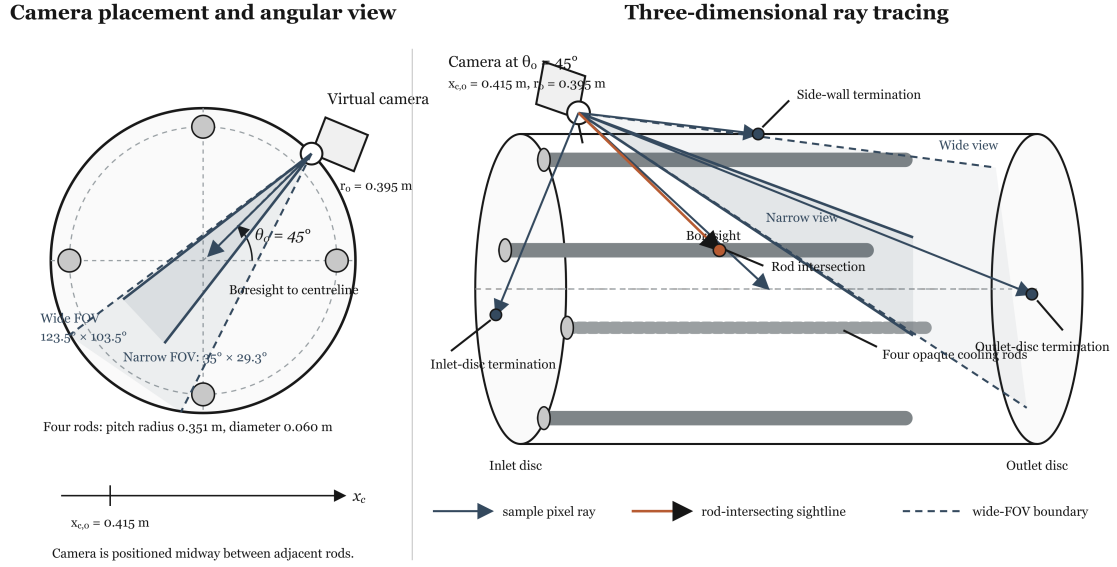


Figure 3.7: Virtual-camera location, field of view, and ray geometry. The schematic shows the camera at $\theta_0 = 45^\circ$, its centreline boresight, the wide and narrow viewing configurations, the four cooling rods, and representative lines of sight through the cylindrical domain.

were integrated towards the camera. Transparent-rod calculations were used only during early code diagnosis and are not part of the reported operating-condition comparisons.

3.4.5 Statistical narrow-band properties

Gas spectral properties were available on 449 bands with centres from 50 to 11250 cm^{-1} and a uniform width of 25 cm^{-1} . The selected 1–5 μm camera window spans 2000–10000 cm^{-1} , so 321 band centres were integrated. Tabulated SNBM parameters were interpolated linearly between 100 K temperature levels. The available tables covered temperatures above 300 K and below 5000 K. For each species and band, the tables supplied a mean absorption parameter κ and an inverse mean line-spacing parameter δ^{-1} .

For a homogeneous path segment of length L_j , the optical amount of species i was

$$X_{i,j} = x_{i,j} \left(\frac{P}{P_{\text{ref}}} \right) L_j 100, \quad P_{\text{ref}} = 101300 \text{ Pa}, \quad (3.19)$$

where the factor 100 converts metres to centimetres. Total pressure was set to 101300 Pa. Oxygen broadening was set to zero in the camera model, consistently with the implemented participating-gas branch.

At $T_s = 296 \text{ K}$ and $P_s = 1 \text{ atm}$, the pressure-broadening parameters used in the

code were

$$\gamma_{\text{H}_2\text{O}} = \frac{P}{P_s} \left[0.462x_{\text{H}_2\text{O}} \frac{T_s}{T} + \left(\frac{T_s}{T} \right)^{1/2} \{0.0792(1 - x_{\text{CO}_2} - x_{\text{O}_2}) + 0.106x_{\text{CO}_2} + 0.036x_{\text{O}_2}\} \right], \quad (3.20)$$

$$\gamma_{\text{CO}_2} = \frac{P}{P_s} \left(\frac{T_s}{T} \right)^{0.7} [0.07x_{\text{CO}_2} + 0.058(1 - x_{\text{CO}_2} - x_{\text{H}_2\text{O}}) + 0.1x_{\text{H}_2\text{O}}]. \quad (3.21)$$

The Curtis–Godson accumulation combined non-uniform cells along a ray. For a given band and species,

$$KX = \sum_j \kappa_j X_j, \quad (3.22)$$

$$K\gamma = \sum_j \kappa_j X_j \gamma_j \delta_j^{-1}, \quad (3.23)$$

$$\beta = \frac{K\gamma}{KX}, \quad (3.24)$$

$$\tau = \exp \left[-2\beta \left(\sqrt{1 + \frac{KX}{\beta}} - 1 \right) \right]. \quad (3.25)$$

For zero optical amount, τ was set to unity. Water-vapour properties were applied over the full tabulated band set, while carbon-dioxide absorption was combined with water vapour in the overlapping bands. The mixture transmissivity was obtained by multiplying the species transmissivities.

3.4.6 Radiative-transfer integration and image formation

The spectral black-body intensity was calculated from Planck’s law in wavenumber form,

$$B_\eta(T) = \frac{1.191066 \times 10^{-8} \eta^3}{\exp(1.4388\eta/T) - 1}, \quad (3.26)$$

where η is in cm^{-1} , giving B_η in $\text{W m}^{-2} \text{sr}^{-1} (\text{cm}^{-1})^{-1}$. The terminating wall or rod provided the initial intensity

$$I_{\eta,0} = \varepsilon_w B_\eta(T_w), \quad \varepsilon_w = 0.9. \quad (3.27)$$

For each gas layer j , traversed from the terminating surface towards the camera, the no-scattering radiative-transfer recurrence was

$$I_{\eta,j} = I_{\eta,j-1} \tau_{\eta,j} + B_\eta(T_j) (1 - \tau_{\eta,j}). \quad (3.28)$$

The intensity assigned to a pixel was the band-integrated value at the camera,

$$I_{\text{pixel}} = \sum_{b \in \text{window}} I_{\eta_b, N} \Delta \eta_b. \quad (3.29)$$

Images were assembled from the 50×50 pixel array and displayed with a common orientation by reversing both plotting axes. Numerical arrays, ray-termination data, intensity fields, and run settings were stored together so that image appearance was not the only retained result.

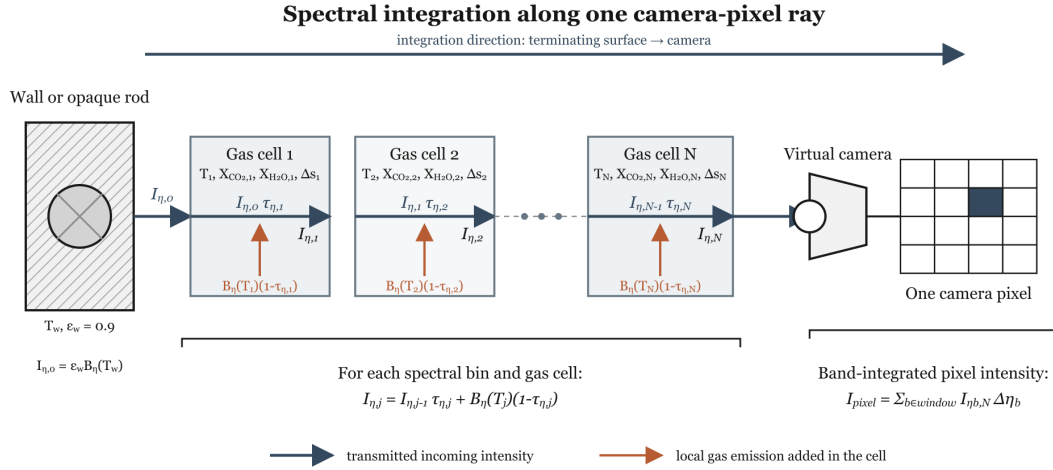


Figure 3.8: Layer-by-layer spectral radiative-transfer calculation along a camera ray. Radiation emitted by the terminating wall or cooling rod is successively attenuated and augmented by gas emission in each traversed cell before spectral-band integration at the camera pixel.

3.4.7 Camera-model numerical checks

Implementation-equivalence, ray-step, and interpolation-grid checks were performed before the images were interpreted. Their numerical details and figures are reported separately in Appendix C. The checks showed that the ray-marching increment was adequate for the tested view, whereas the camera interpolation was not fully grid independent. Quantitative interpretation therefore uses the refined grid, and the remaining post-processing uncertainty is kept separate from the CFD mesh assessment.

3.5 Post-processing and comparison procedure

CFD results were post-processed using a consistent set of planes, profiles, and integral quantities. Temperature, velocity, oxygen, carbon monoxide, carbon dioxide, and water-vapour fields were examined on longitudinal and transverse planes. The recirculation zone was identified from the axial-velocity sign and streamline topology. Model comparisons used identical colour ranges and sampling coordinates. Where experimental and numerical data were paired, the error at location n was defined as

$$e_n = \phi_{CFD,n} - \phi_{exp,n}, \quad (3.30)$$

and summarised, when sufficient points were available, by the mean absolute error

$$MAE = \frac{1}{N} \sum_{n=1}^N |e_n|. \quad (3.31)$$

The error metric was interpreted together with the spatial profiles and flame structure rather than as a stand-alone ranking.

Camera cases were compared using band-integrated pixel intensity, image mean, selected percentiles, spatial intensity profiles, and the fractions of rays terminating at each surface type. The same camera position, spectral window, field of view, wall emissivity, and colour scale were retained when an operating parameter was compared. This ensured that image differences arose from the CFD fields and not from post-processing settings.

3.6 Methodology summary

The adopted methodology retained the burner features that control swirl and mixing, applied local polyhedral-mesh refinement to those features, and used the same 2.096-million-cell grid for the turbulence comparison. Reacting-flow calculations coupled species transport, EDC, the Jones–Lindstedt UDF, DO radiation, and WSGGM gas properties. The assessed model was then applied to a structured matrix of excess-air ratios, fuel flows, and primary/secondary air splits. Finally, CFD temperature and participating-gas fields were transferred to a cylindrical SNBM ray tracer that included furnace-wall emission, cooling rod occlusion, and wavelength-resolved gas emission and absorption. Keeping the CFD radiation model and the camera radiation model as separate, explicitly verified stages made it possible to trace synthetic-image changes back to the underlying flow solution and operating condition.

4

Results

This chapter first assesses the reference CFD solution against the published pure-propane O_2 and CO measurements. The operating studies then follow a consistent sequence: local species fields and profiles are interpreted before the corresponding line-of-sight infrared images. Experimental data are used as a reference assessment at the nominal operating condition; elsewhere they provide context rather than a claim of validation. Because the reconstructed numerical geometry includes the Chalmers cooling rods, even the nominal case is not treated as an exact reproduction of the experimental configuration. Detailed numerical-resolution checks are reported in Appendix C.

4.1 Reference oxygen and CO assessment at $\lambda = 1.15$

The experimental reference is the 100% propane flame of Colin et al. [1], operated at approximately 80 kW and $\lambda = 1.15$. Figure 4.1 reproduces the published CO and O_2 contour panels and compares them with the present 41.15/58.85 calculation. Both species use the paper’s original limits— 0–6 vol.% CO and 0–10 vol.% O_2 —so colour represents the same concentration in each experimental/CFD pair. Values above a limit are saturated rather than rescaled.

The experiment and CFD agree on the coupled topology: CO is concentrated in a central region from which O_2 is depleted, while oxygen-rich shoulders form on either side of the core. Their magnitudes and downstream development differ. O_2 is reported together with CO because the two fields distinguish oxidiser penetration from incomplete conversion. CO receives particular attention as a mixing- and chemistry-sensitive intermediate, while camera intensity is governed directly by temperature and the radiating products CO_2 and H_2O , not by CO alone. The experimental CO column narrows and weakens strongly from M2 to M5; the CFD retains a longer saturated core, with its maximum decreasing from about 11.42 vol.% at M2 to 3.30 vol.% at M5. The corresponding experimental centreline average decreases from about 3.68 to 0.17 vol.%. O_2 provides the complementary evidence: the experiment has two strong M2 lobes, reaching about 13.75 vol.% on average, whereas the calculated M2 maximum is only about 5.79 vol.%. Too little O_2 in the shear-layer shoulders together with too much CO in the centre indicates under-resolved fuel–air mixing or an overly persistent rich reaction zone, rather than a uniform concentration offset.

Figure 4.2 tests the same structure along the 30, 35, and 40 cm axial sampling lines.

CO and O₂ contour comparison
 Paper: 100% propane, $\lambda = 1.15$, no transport air; Fluent: 100% propane, 41%/58% split of 31.01 g/s air

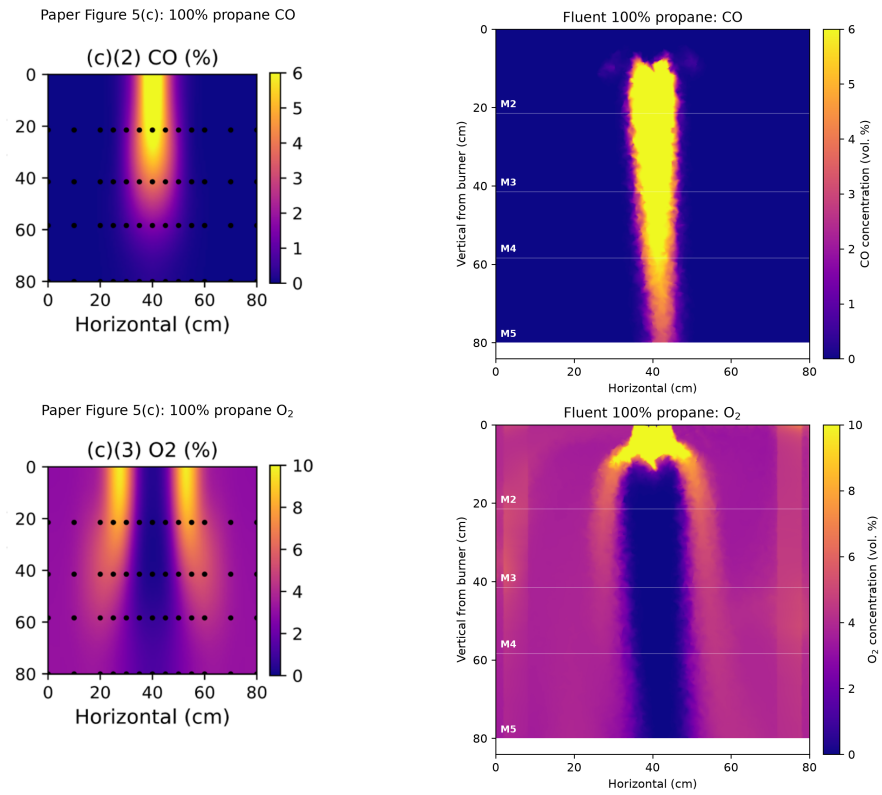


Figure 4.1: Published pure-propane CO and O₂ contours from Colin et al. [1] compared with the present CFD result at $\lambda = 1.15$. The 41/58 identifier denotes the primary/secondary combustion-air split, not fuel composition.

On the 30 cm line, both retained O_2 solutions reproduce the rise and decay but underpredict the first measurements. At 35 and 40 cm, the near-burner O_2 peak collapses before M2 and the low downstream values are captured qualitatively; the separation between the RNG $k-\varepsilon$ and SST $k-\omega$ curves, especially at 35 cm, shows that radial transport remains turbulence-model sensitive. The CO profiles locate the same deficiency from the product side. The calculation produces a narrow near-burner peak at 30 cm and broader CO-rich regions at 35 and 40 cm. The 40 cm profile follows the measured downstream decline more closely, while the 35 cm profile overpredicts both the near-burner level and its persistence.

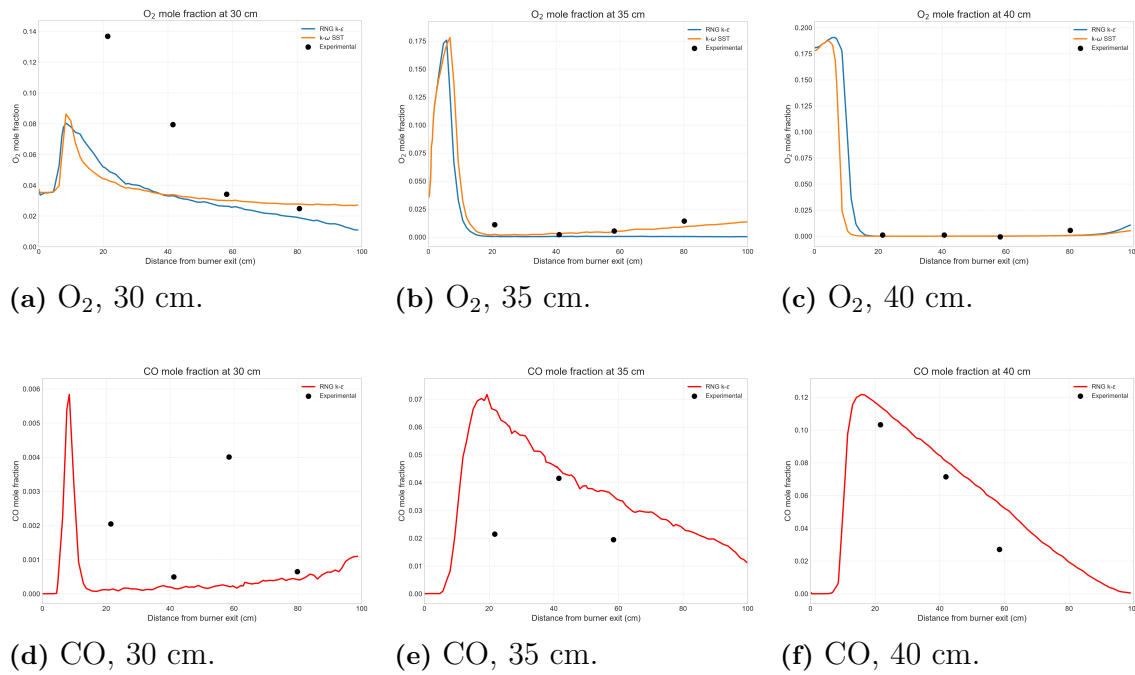


Figure 4.2: Axial O_2 and CO mole-fraction profiles for the reference propane flame. Symbols are the 2024 measurements and curves are extracted from the Fluent solution.

The M2–M5 radial comparison in Figure 4.3 gives equal weight to oxidiser penetration and CO conversion. Calculated CO peaks decrease monotonically from 11.42, through 8.42 and 6.00, to 3.30 vol.% at M2–M5, respectively, so the model predicts the correct downstream ordering but not the measured rate of decay. The O_2 profiles reproduce centreline depletion and improve outside the core at downstream stations, but miss the amplitude and abrupt radial gradient of the experimental M2 shoulders. Taken together, the axial and radial comparisons support use of the model for topology and parametric trends, while ruling out an interpretation of the calculated concentrations as fully quantitative validation data.

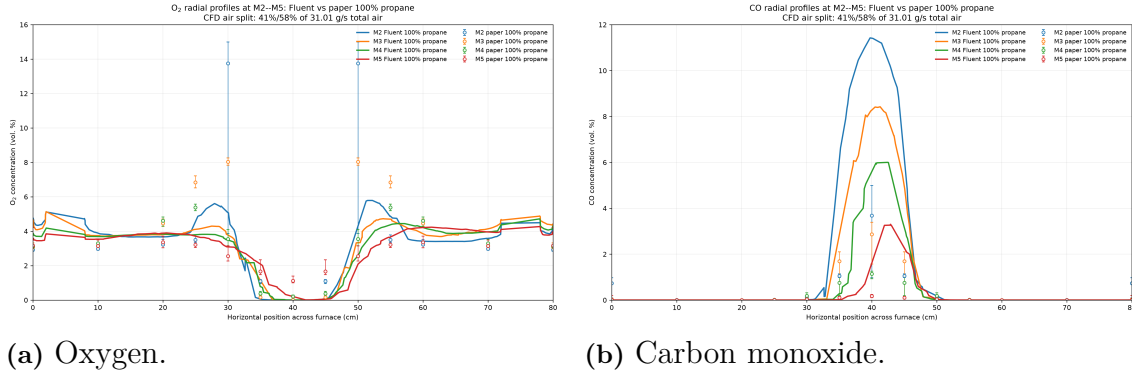


Figure 4.3: Radial O₂ and CO profiles at M2–M5. Curves show CFD; symbols and ranges show the reconstructed experimental averages and minimum-to-maximum intervals from Colin et al. [1].

4.2 Effect of primary-to-secondary air distribution at $\lambda = 1.15$

The following comparison isolates redistribution of the oxidiser between the two swirl passages. The propane flow, total air flow, and hence the global excess-air ratio were unchanged; only the primary/secondary percentages were varied according to Equation 3.14. Consequently, differences between cases should be interpreted as effects of inlet momentum, swirl, and near-field mixing rather than as changes in global mixture strength.

The species and temperature contours show the central longitudinal plane over the first 80 cm downstream of the burner. The horizontal centreline is at 40 cm, and the black points identify the M2–M5 sampling rows. Fixed ranges of 0–10 vol.% for O₂, 0–6 vol.% for CO, and 284–2233 K for temperature were applied to all six cases. Values above a concentration range therefore appear at the upper colour without implying that they are equal. Only plots containing both CFD and experimental results are included below; the separate experimental-only mean, minimum/maximum, and standard-deviation plots are not repeated.

The measurements were obtained for the reference 41.15/58.85 split [1]. They are therefore the closest available reference for that case, but the geometry difference described in Section 3.3.5 precludes a strict matched-validation claim. In the other five cases the same points are retained as a common reference to show how far the predicted field moves when the air is redistributed; agreement with those points must not be interpreted as validation of an unmeasured air split. Table 4.1 provides quantitative support for the visual comparisons. The area fractions are two-dimensional measures on the plotted plane, not furnace-volume fractions. The profile errors are mean absolute differences from the experimental averages at all plotted M2–M5 positions and are reported in concentration percentage points.

Table 4.1: Summary measures for the primary/secondary air-split cases at $\lambda = 1.15$.

Split primary/secondary	$A_{O_2 < 1\%}$ (%)	$A_{CO > 1\%}$ (%)	$T_{\max}$ (K)	$A_{T \geq 1800\text{ K}}$ (%)	MAE_{O_2} (p.p.)	MAE_{CO} (p.p.)
41.15/58.85	13.71	13.09	2138	9.65	1.25	0.81
58.85/41.15	10.72	6.52	2233	11.39	1.14	0.23
10/90	13.14	13.27	2067	7.20	1.30	0.85
90/10	2.34	1.50	2168	4.38	1.58	0.32
25/75	13.47	13.75	2087	8.60	1.35	0.95
75/25	5.28	2.78	2215	8.59	1.22	0.26

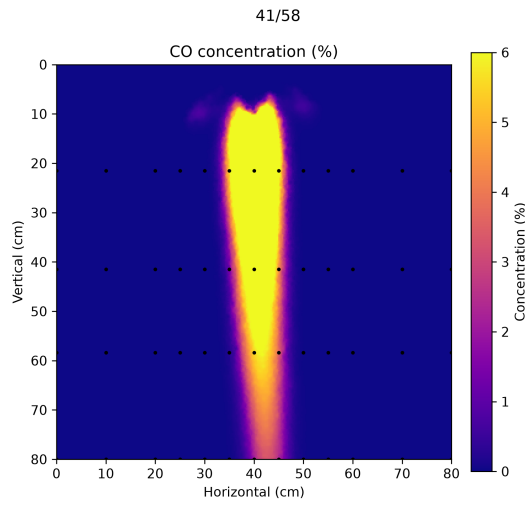
4.2.1 Near-balanced air splits

Figure 4.4 shows that the reference 41.15/58.85 case formed a long oxygen-depleted core around the furnace centreline. A co-located CO-rich column persisted through M2, M3, and M4 and remained visible towards M5. Reversing the near-balanced split to 58.85/41.15 retained the central oxygen deficit but shortened the high-CO region markedly: the area with CO above 1 vol.% decreased from 13.09 to 6.52% of the plotted plane. The oxygen-depleted area decreased more moderately, from 13.71 to 10.72%. Thus, the principal change was not removal of the fuel-rich core but earlier conversion of CO within it.

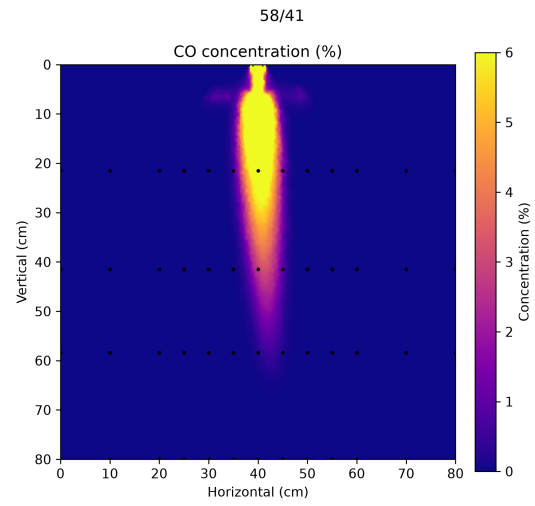
The temperature fields in Figure 4.5 are consistent with this change in oxidation pattern. The reference case retained two hot shear-layer branches around a cooler inlet core and a comparatively long, moderately hot central column. With the larger primary-air fraction, the branches merged closer to the burner and produced a broader high-temperature zone. The maximum temperature increased by 95 K and the area above 1800 K increased from 9.65 to 11.39%. Since the total oxidiser flow was fixed, this is most consistently explained by improved early contact between the central fuel jet and the adjacent primary-air stream, together with the associated change in swirl-generated transport. The secondary passage is farther from the fuel injector; allocating more air there leaves a richer central path and shifts part of the final CO oxidation downstream.

The radial profiles in Figure 4.6 clarify the model-measurement differences that are compressed in the contours. Both the reference CFD solution and the measurements identify an oxygen-poor centre, but the CFD underpredicts the two oxygen-rich shoulders measured near the edges of the inner mixing layer at M2. The experimental M2 average reaches approximately 13.2 vol.% at the shoulders, whereas the reference CFD peak is approximately 5.9 vol.%. At the same time, the reference simulation overpredicts the CO-rich core: its M2 centreline peak is about 11.5 vol.%, compared with an experimental average of 3.60 vol.% and an extracted maximum of 4.89 vol.%. The excessive CFD CO peak remains evident at M3–M5. This paired behaviour—too little oxygen in the shear-layer shoulders and too much persistent CO in the centre—indicates insufficient resolved mixing or over-persistent rich chemistry in the steady RANS prediction, rather than a simple uniform concentration offset.

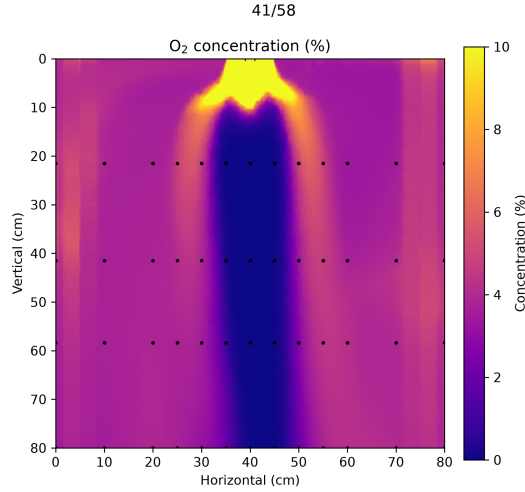
The 58.85/41.15 solution narrows and lowers the downstream CO peaks and gives a smaller numerical CO MAE against the reference points. However, it also reduces



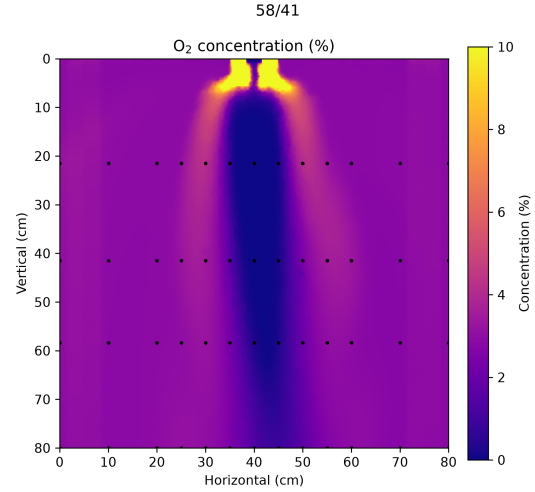
(a) 41.15/58.85: CO.



(b) 58.85/41.15: CO.



(c) 41.15/58.85: O₂.



(d) 58.85/41.15: O₂.

Figure 4.4: CO and oxygen contours for the near-balanced air distributions. The common upper limits are 6 vol.% CO and 10 vol.% O₂.

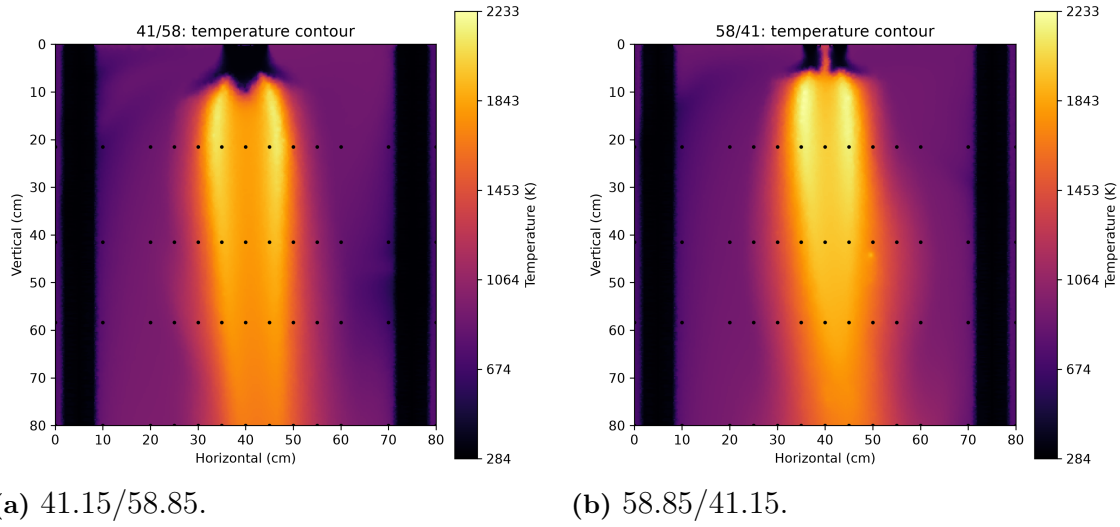


Figure 4.5: Temperature contours for the near-balanced air distributions, shown on the common 284–2233 K scale.

the oxygen shoulders and does not reproduce the large measured M2 oxygen peaks. Its smaller CO error is therefore evidence of the parametric sensitivity, not evidence that the reversed split represents the experiment.

The synthetic IR images in Figure 4.7 integrate emission and attenuation along each camera ray, principally through the hot H_2O - and CO_2 -containing products. They are not local temperature maps. The image view and the longitudinal concentration contours both place the burner at the top. The vertical low-intensity bands are caused mainly by the opaque cooling rods and associated line-of-sight obstruction, while the central bright column marks the radiating product region. The reference case shows a comparatively extended bright column, consistent with its elongated CO-rich and hot core. The 58.85/41.15 case concentrates the strongest signal near the burner-facing part of the view and has a more uniform, weaker downstream column, consistent with earlier heat release and CO conversion. All camera images use the common $0\text{--}15,000 \text{ W m}^{-2} \text{ sr}^{-1}$ colour scale, so both spatial structure and radiance magnitude can be compared directly between panels.

4.2.2 Extreme distributions: 10/90 and 90/10

The extreme pair produced the clearest separation between the two combustion regimes. In the 10/90 case, Figure 4.8 shows an oxygen-depleted central column and CO above the 6 vol.% plotting limit over a large part of the first 60 cm. In the 90/10 case, the high-CO region is restricted to the immediate burner zone and is essentially absent at M3–M5. The plane area above 1 vol.% CO falls from 13.27 to 1.50%, while the area below 1 vol.% oxygen falls from 13.14 to 2.34%. The inverse CO–oxygen relationship confirms that the long CO column is associated with a locally rich, oxygen-starved path rather than with uniformly slow CO oxidation over the whole furnace.

The corresponding temperature contours in Figure 4.9 distinguish peak temperature

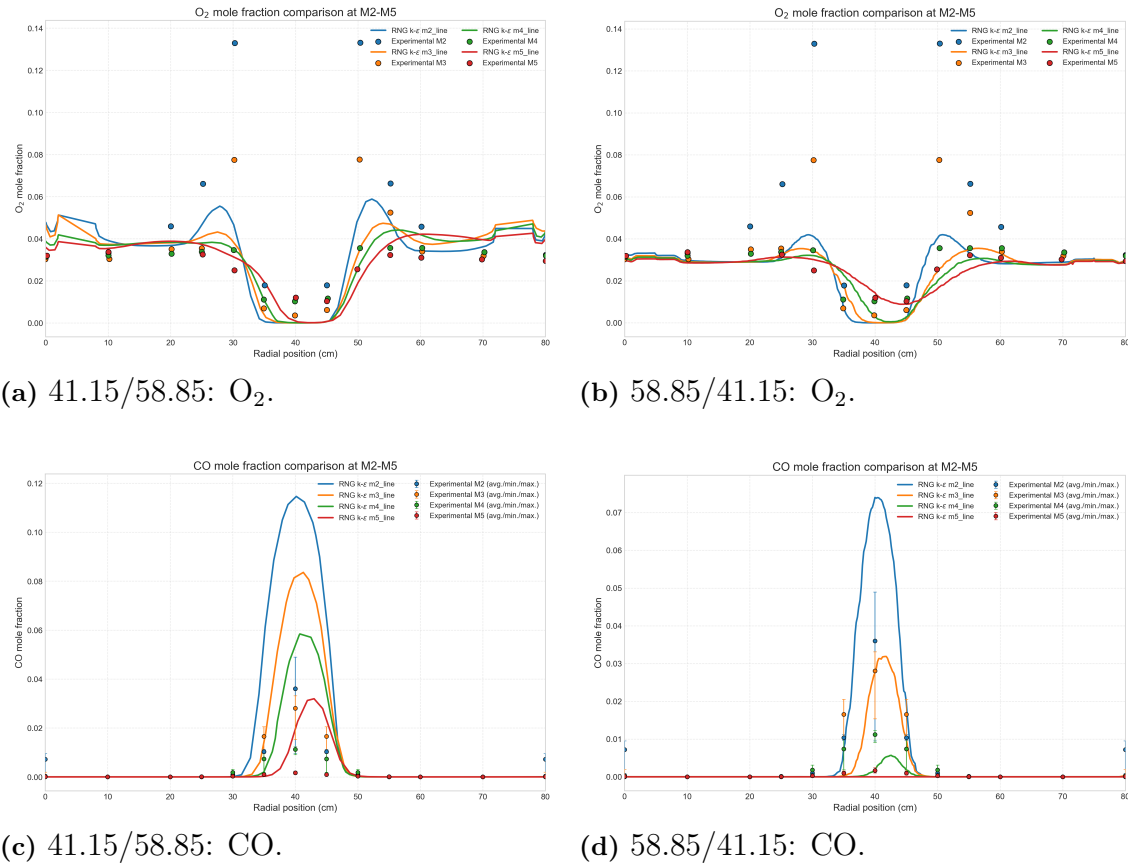


Figure 4.6: CFD and experimental radial species profiles at M2–M5 for the near-balanced distributions. Markers denote experimental averages; the CO error bars span the extracted minimum and maximum values. The experimental data correspond to the 41.15/58.85 operating condition.

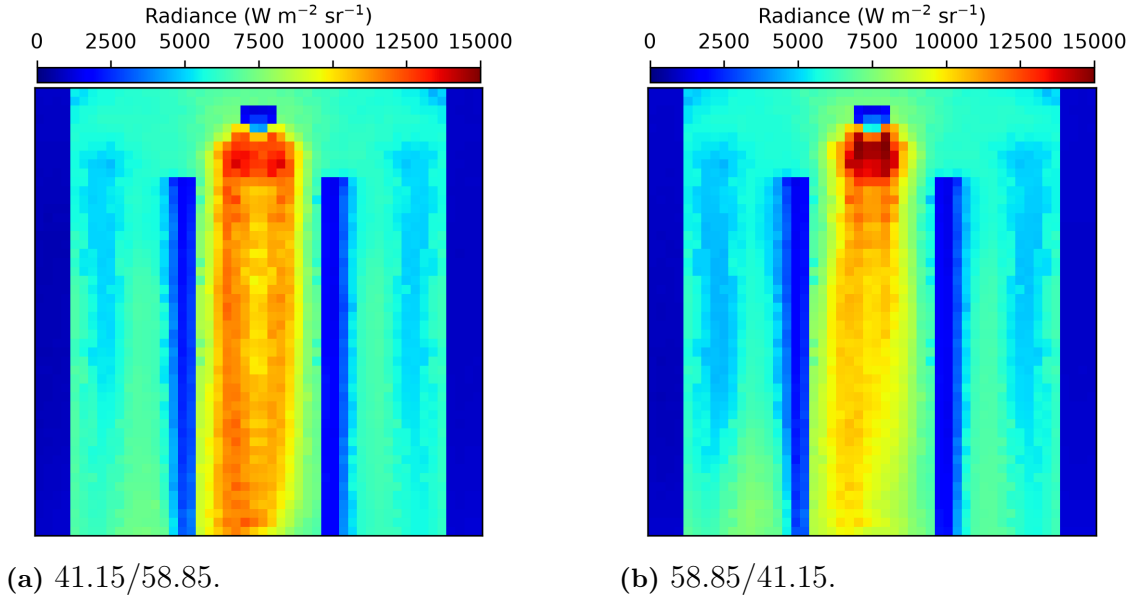
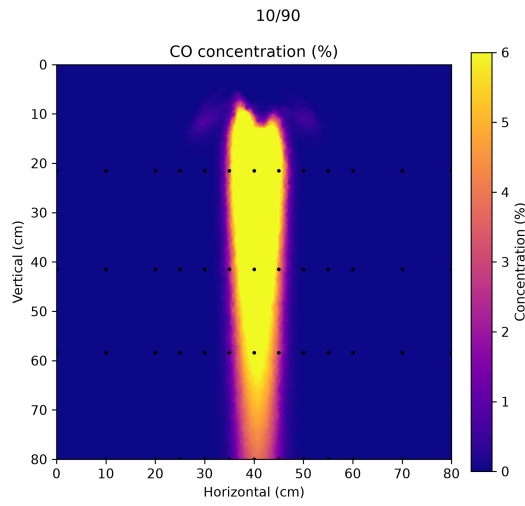


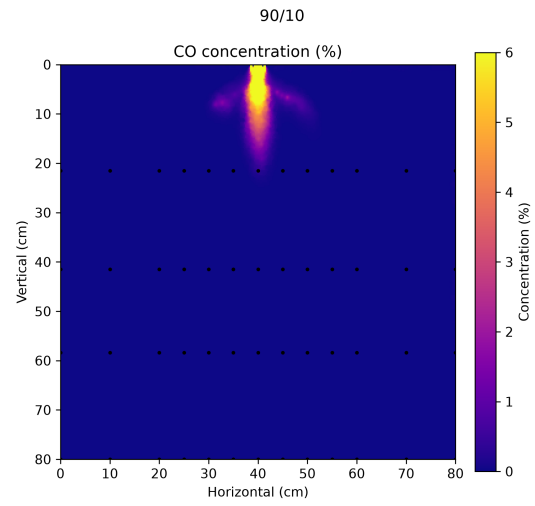
Figure 4.7: Synthetic band-integrated IR radiance for the near-balanced air distributions, shown on the common $0\text{--}15,000\text{ W m}^{-2}\text{ sr}^{-1}$ radiance scale.

from the spatial extent of the hot zone. The 10/90 solution forms two hot branches around a cool central inlet region and carries a moderately hot core far downstream. Its maximum temperature is 2067 K and 7.20% of the plotted plane is above 1800 K. The 90/10 case reaches a higher local maximum of 2168 K but has only 4.38% of the plane above 1800 K; the hottest region is compact and close to the burner. Directing 90% of the air through the primary annulus therefore intensifies early fuel–air contact but consumes and dilutes the reacting mixture over a shorter distance. Directing 90% through the outer secondary passage delays that contact, giving a longer but less intense reaction zone.

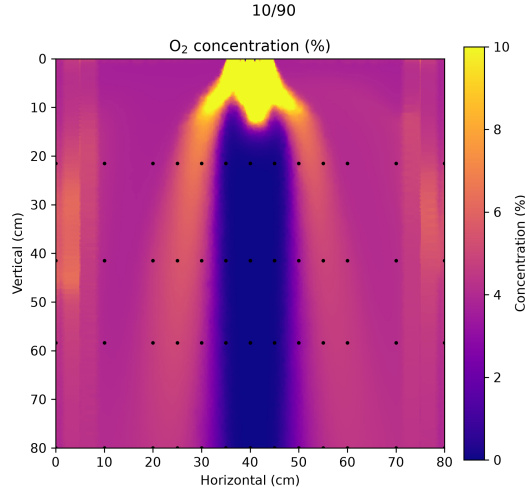
Figure 4.10 shows the same transition in radial form. At 10/90, the CFD profiles retain high, narrow CO peaks and near-zero centreline oxygen through the downstream probes, closely resembling the qualitative structure of the reference 41.15/58.85 simulation. At 90/10, the CO peak has largely disappeared by M4 and M5, while oxygen penetrates the central region earlier. Relative to the reference measurements, this produces a lower CO MAE but a larger oxygen MAE (0.32 and 1.58 percentage points, respectively) than the 10/90 case (0.85 and 1.30 percentage points). These opposite changes are physically consistent: faster oxidation removes CO but also fills the experimentally oxygen-poor core too early. Because neither extreme split was measured, the error values describe displacement from the reference experiment rather than predictive accuracy for the extreme cases.



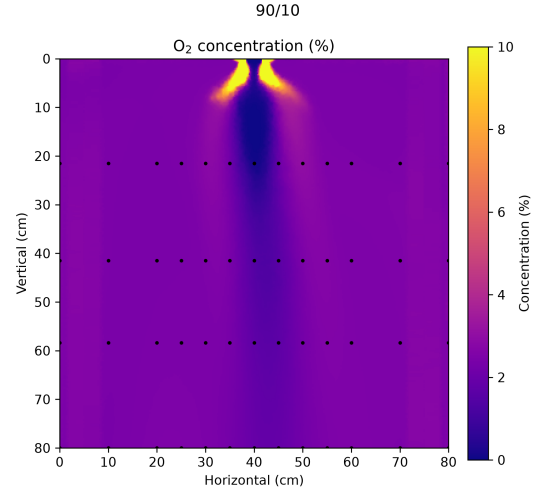
(a) 10/90: CO.



(b) 90/10: CO.



(c) 10/90: O₂.



(d) 90/10: O₂.

Figure 4.8: CO and oxygen contours for the extreme air distributions, using the common 0–6 and 0–10 vol.% scales, respectively.

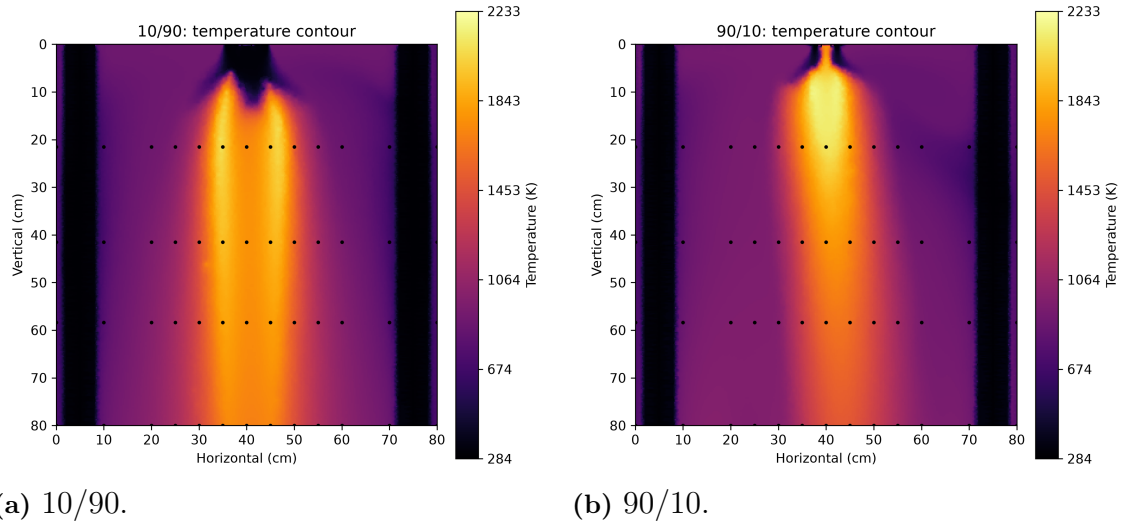


Figure 4.9: Temperature contours for the extreme air distributions, shown on the common 284–2233 K scale.

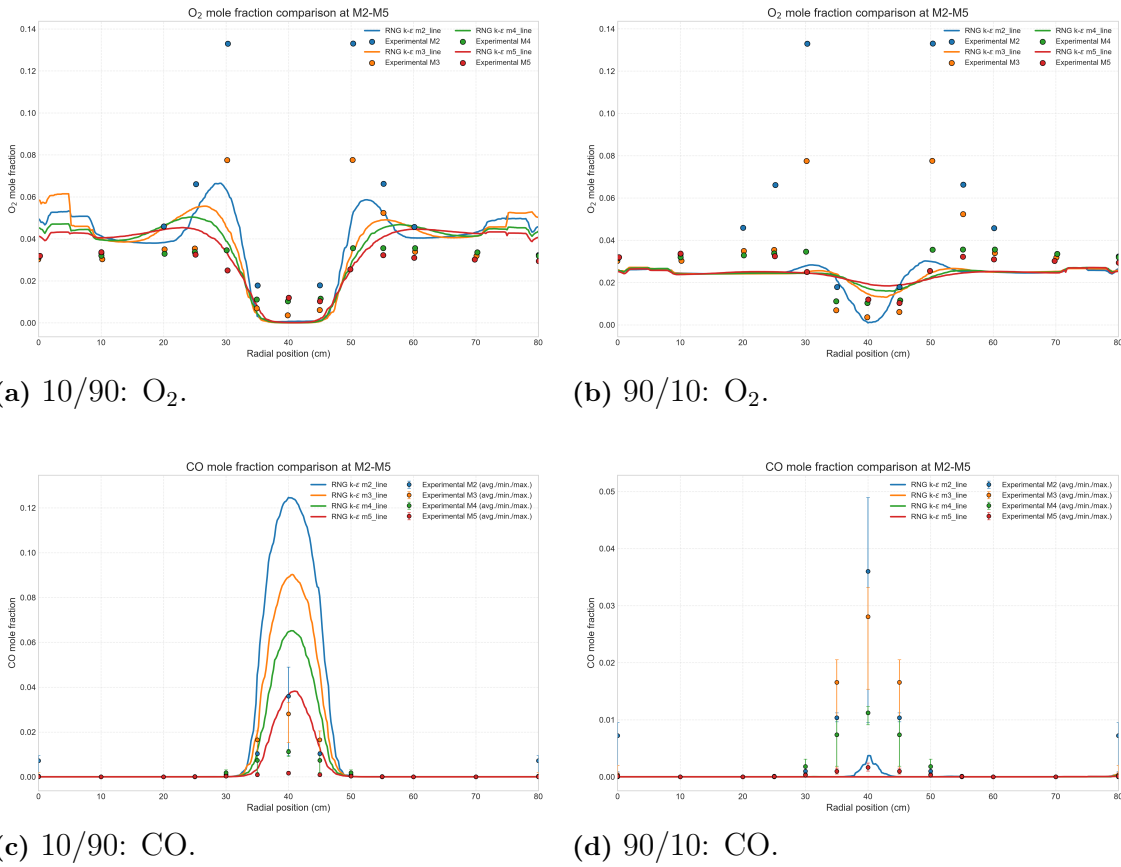


Figure 4.10: CFD and reference experimental radial species profiles at M2–M5 for the extreme air distributions. The measurements correspond to the 41.15/58.85 split and are shown only as a common benchmark.

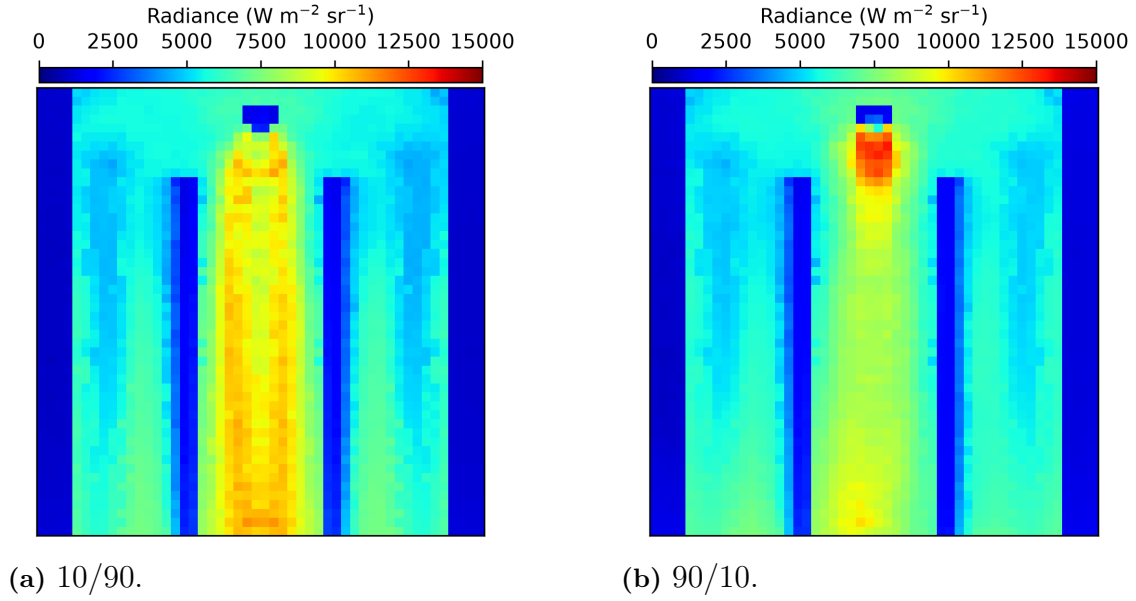


Figure 4.11: Synthetic band-integrated IR radiance for the extreme air distributions, shown on the common $0\text{--}15,000 \text{ W m}^{-2} \text{sr}^{-1}$ radiance scale.

The IR images in Figure 4.11 reproduce the spatial contrast seen in the CFD fields. The 10/90 case gives a continuous bright central column over most of the visible furnace length. The 90/10 case gives a compact high-intensity region near the burner-facing end and a much less pronounced downstream column. This agreement between the line-of-sight image, the local temperature field, and the CO/oxygen topology strengthens the interpretation of delayed mixing at 10/90 and concentrated early heat release at 90/10. The common colour scale also permits direct comparison of their radiance magnitudes.

4.2.3 Intermediate distributions: 25/75 and 75/25

The intermediate pair follows the same trend while avoiding the most extreme inlet redistribution. Figure 4.12 shows that 25/75 retains a long, narrow CO-rich column embedded in a broad oxygen-depleted core. At 75/25, the CO-rich region contracts towards the burner and the downstream oxygen field becomes much more uniform. The area above 1 vol.% CO decreases from 13.75 to 2.78%, and the oxygen-depleted area decreases from 13.47 to 5.28%. The close similarity between the 25/75, 10/90, and reference species fields indicates that once the secondary passage carries most of the air, further redistribution within that secondary-rich regime changes the length and width of the rich core less than reversing which passage is dominant.

The temperature comparison in Figure 4.13 is particularly informative. Both cases have almost the same plane fraction above 1800 K (8.60 and 8.59%), yet their distribution is different. The 25/75 case has a lower maximum temperature of 2087 K and spreads the hot zone along two shear-layer branches and a long central column. The 75/25 case reaches 2215 K and concentrates more of the highest temperature close to the burner before the field broadens downstream. The air split therefore

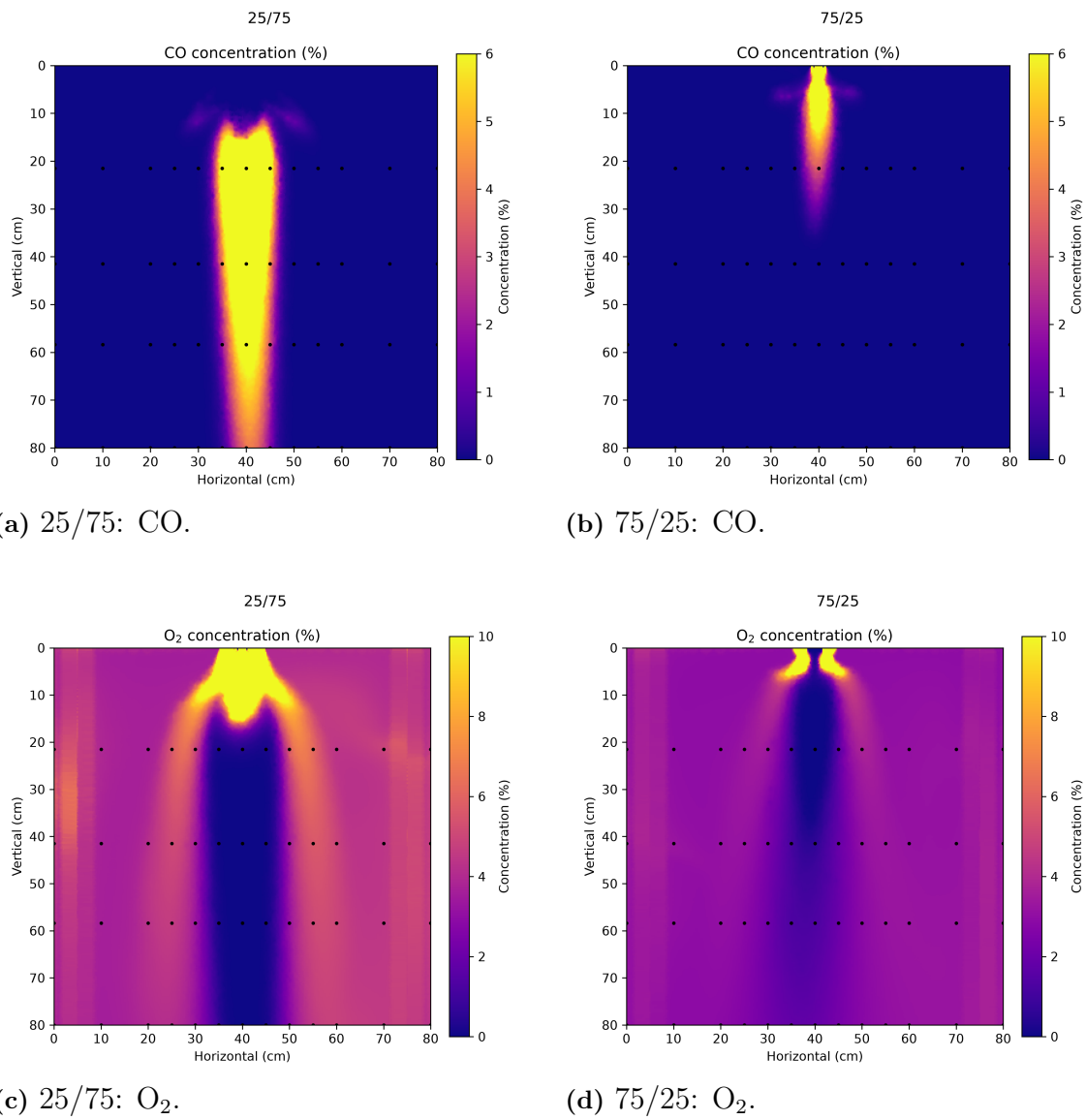


Figure 4.12: CO and oxygen contours for the intermediate air distributions, using the common 0–6 and 0–10 vol.% scales, respectively.

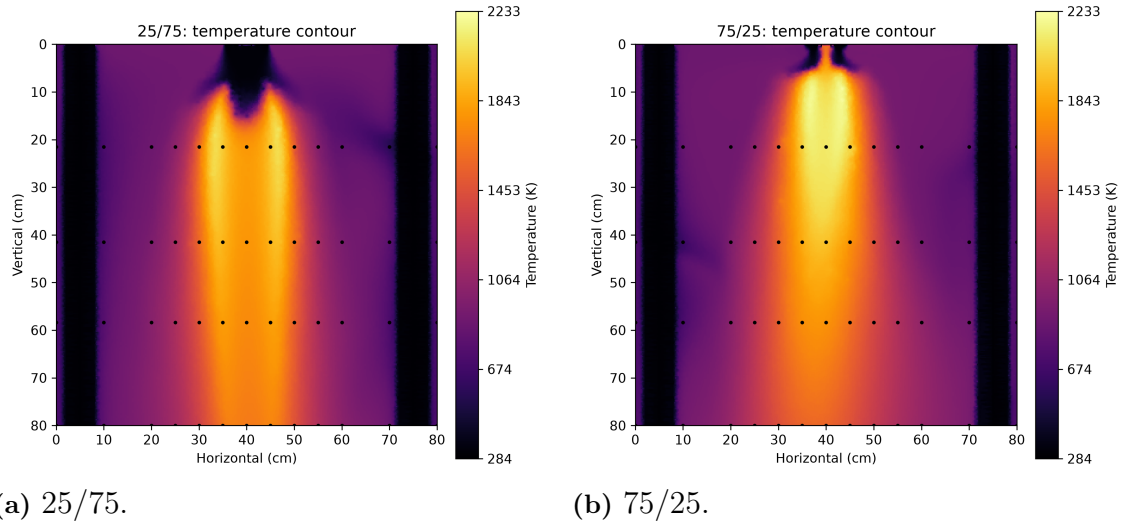
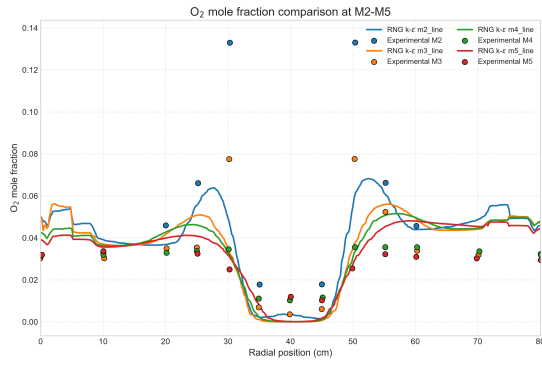
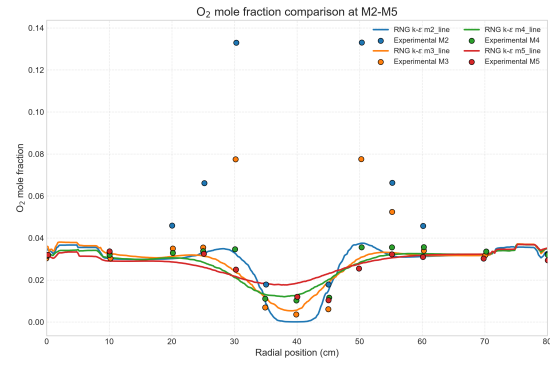
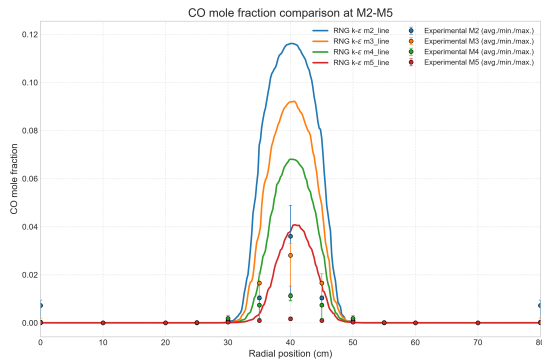


Figure 4.13: Temperature contours for the intermediate air distributions, shown on the common 284–2233 K scale.

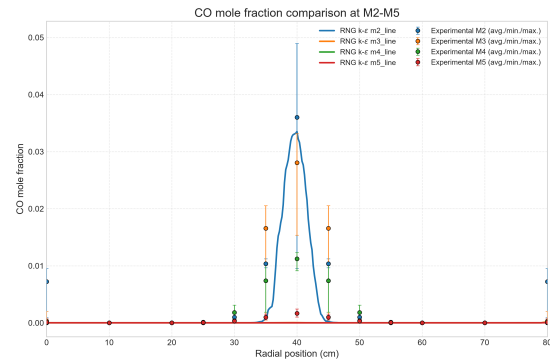
redistributes heat release in space even when a threshold-based hot-area measure remains unchanged. This is consistent with faster near-field mixing through the primary passage and slower entrainment of outer secondary air into the fuel core. The M2–M5 profiles in Figure 4.14 demonstrate how this spatial redistribution affects the validation observables. At 25/75, the predicted CO core remains too high at all four rows relative to the reference measurements, while the measured oxygen-rich M2 shoulders remain underpredicted. At 75/25, the CO peak decays rapidly downstream and the centreline oxygen recovers earlier. The resulting CO MAE decreases from 0.95 to 0.26 percentage points, whereas the oxygen MAE changes from 1.35 to 1.22 percentage points. The modest oxygen change compared with the large CO change shows that CO is the more sensitive indicator of the modelled residence time and local rich-zone persistence. Again, the lower errors at 75/25 do not constitute validation because the comparison points were measured at the reference split.

The synthetic images in Figure 4.15 provide the same qualitative ordering. The 25/75 result contains an extended central radiance column, whereas the 75/25 result is dominated by a compact near-burner maximum and a weaker downstream column. The dark rod shadows remain in the same locations because camera geometry and opaque-surface treatment are unchanged; changes between the central columns therefore originate from the CFD temperature and radiating-species fields rather than from camera placement. Because the panels use the same colour bar, equal colours represent equal radiance and the intensity difference is directly comparable.

Across all three pairs, increasing the primary-air fraction consistently contracts the oxygen-depleted and CO-rich core and moves the strongest heat release closer to the burner. Increasing the secondary-air fraction produces a longer rich core, prolonged CO, and a spatially extended but generally lower-peak hot zone. These trends are consistent with the primary annulus coupling oxidiser directly to the central

(a) 25/75: O_2 .(b) 75/25: O_2 .

(c) 25/75: CO.



(d) 75/25: CO.

Figure 4.14: CFD and reference experimental radial species profiles at M2–M5 for the intermediate air distributions. The measurements correspond to the 41.15/58.85 split and are shown only as a common benchmark.

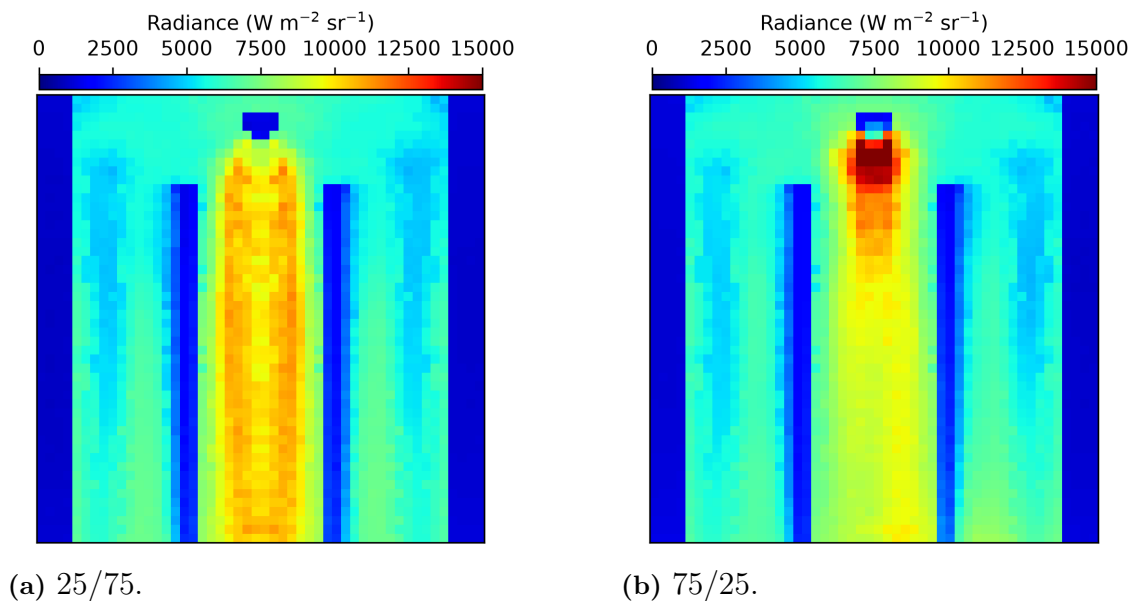


Figure 4.15: Synthetic band-integrated IR radiance for the intermediate air distributions, shown on the common 0–15,000 W m⁻² sr⁻¹ radiance scale.

fuel jet, while the outer secondary stream must be transported inward by swirl, shear-layer entrainment, and recirculation. The present contours do not contain velocity or residence-time diagnostics, so the relative contributions of momentum, swirl number, and recirculation strength cannot be separated from these results alone. The conclusions are therefore stated as coupled mixing-and-chemistry trends rather than as a unique flow-mechanism identification. This interpretation is also consistent with the reported sensitivity of non-premixed swirl flames to the primary-air momentum ratio and swirl-induced recirculation [4, 7].

4.3 Effect of excess-air ratio on oxygen and carbon monoxide

The interaction between global excess-air ratio and primary/secondary air distribution was assessed by comparing the six air splits at $\lambda = 0.60$, 1.00, 1.15, and 1.623. Figures 4.16–4.18 use the same 0–6 vol.% CO and 0–10 vol.% O₂ ranges for all 24 cases. The comparison therefore shows both changes in plume topology and changes in concentration level without rescaling each operating point. Values above the upper limits are clipped to the upper colour. No experimental markers are used for $\lambda = 0.60$, 1.00, or 1.623 because measurements were not available at those excess-air ratios. The published $\lambda = 1.15$ contour in Figure 4.1 is therefore the common experimental anchor and is not duplicated beside every parametric panel. The $\lambda = 0.60$ cases are understoichiometric screening cases. They are retained to show where the numerical solution changes branch, but they are not used for quantitative design conclusions. In particular, the 25/75 case exceeds the adopted heat-

balance limit and the primary-dominant 75/25 and 90/10 cases approach weakly reacting or cold states. These cases are identified explicitly below rather than interpreted as physically validated furnace operation.

Two plane-area measures were calculated directly from the plotted fields: the fraction with $\text{O}_2 < 1$ vol.% and the fraction with $\text{CO} > 1$ vol.%. Table 4.2 reports the range across the six air splits. These are two-dimensional measures on the displayed central plane and should not be interpreted as furnace-volume fractions. The very wide range at $\lambda = 0.60$ is physically important: it reflects a transition between strongly reacting, weakly reacting, and non-reacting numerical states rather than an exceptionally strong continuous air-split trend.

Table 4.2: Range of oxygen-depleted and CO-rich plane areas across the six air splits at each excess-air ratio.

Excess-air ratio	$A_{\text{O}_2 < 1\%}$ (%)	$A_{\text{CO} > 1\%}$ (%)
0.60	0.01–97.24	0.00–98.91
1.00	11.58–30.73	5.83–16.98
1.15	2.34–13.71	1.50–13.75
1.623	0.21–2.34	0.73–2.67

4.3.1 Near-balanced distributions

The 41.15/58.85 sequence in Figure 4.16 gives the clearest continuous response to excess air. At $\lambda = 0.60$, a CO-rich central column extends through the full plotted height and is surrounded by a broad oxygen-depleted region. The corresponding plane fractions are 26.74% for CO above 1 vol.% and 47.68% for oxygen below 1 vol.%. At $\lambda = 1.00$, the CO column remains attached to the lower boundary of the plotted domain but becomes narrower; the two area fractions decrease to 16.63 and 17.22%, respectively. Increasing the ratio to 1.15 gives a further, moderate contraction. At $\lambda = 1.623$, CO above 1 vol.% is restricted to the first approximately 25 cm and occupies 2.36% of the plane, while the oxygen-depleted core ends at approximately 31 cm and occupies 1.82%.

This ordering is consistent with the global oxygen balance. The rich cases cannot supply enough oxygen for complete conversion everywhere in the central flow, so CO and oxygen depletion persist downstream. Added air increases the oxygen concentration outside the reaction zone and promotes conversion of CO within a progressively shorter distance. Even at $\lambda = 1.623$, however, the immediate burner region contains a narrow oxygen-poor core and local CO maximum. Global excess oxygen therefore does not imply locally premixed or uniformly lean conditions: finite-rate reaction and the time required for the annular air streams to mix with the fuel still create a locally rich near-field region.

The reversed 58.85/41.15 sequence follows the same ordering for $\lambda = 1.00$, 1.15, and 1.623. CO above 1 vol.% decreases from 8.65 to 6.52 and 1.14% of the plane, respectively, while the CO plume contracts towards the burner. Relative to 41.15/58.85 at the same excess-air ratio, the larger primary fraction generally shortens the CO-rich core, consistent with the primary stream contacting the central fuel jet more directly.

The $\lambda = 0.60$, 58.85/41.15 result is a marked exception. Almost the entire plane is oxygen-depleted (97.24%) and above 1 vol.% CO (98.91%), with a plane-mean CO concentration of 5.61 vol.%. The associated temperature field reaches 2108 K, confirming that this is a reacting result rather than a cold-flow solution. It nevertheless represents extremely incomplete oxidation over the displayed domain. This single case must not be used to infer that increasing the primary fraction always raises CO; rather, it shows that the rich operating point can enter a qualitatively different mixing-chemistry state when the inlet momentum distribution is changed.

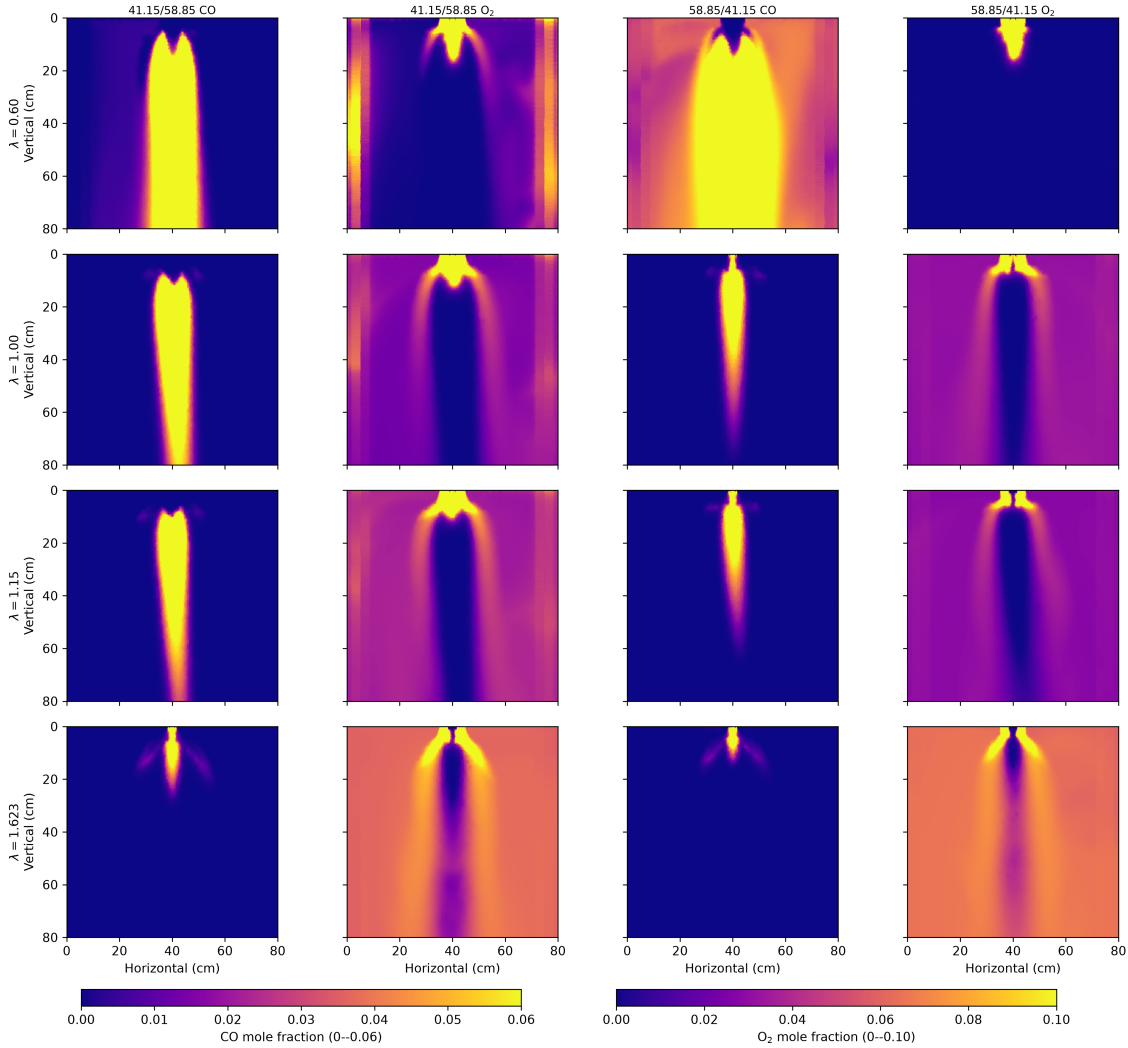


Figure 4.16: CO and oxygen contours for the near-balanced air distributions across the four excess-air ratios. Rows correspond to excess-air ratio and columns to split and species. The fixed ranges are 0–6 vol.% CO and 0–10 vol.% O₂.

4.3.2 Extreme distributions

For the secondary-dominant 10/90 split, Figure 4.17 again shows a continuous change with excess air. The $\lambda = 0.60$ result contains a broad CO-rich core extending through the full 80 cm view. The CO-rich plane fraction decreases from

25.70% at $\lambda = 0.60$ to 16.06% at 1.00, 13.27% at 1.15, and 1.98% at 1.623. The oxygen-depleted area follows the same ordering, decreasing from 46.30 to 16.25, 13.14, and 1.58%. The nested CO-rich and oxygen-poor regions therefore remain coupled over the full range: greater global oxygen availability progressively shortens the rich reaction path, but the high secondary fraction continues to delay inward oxidiser transport relative to the primary-dominant case.

At $\lambda = 1.00$, 1.15, and 1.623, the 90/10 case produces substantially less CO than 10/90. The CO-rich area is 5.83, 1.50, and 0.73%, respectively, and the highest concentrations are increasingly confined to the burner exit. At $\lambda = 1.00$, however, the 90/10 field still has a large oxygen-depleted area of 30.73% even though its CO-rich area is the smallest of the six splits at that excess-air ratio. Near the stoichiometric global condition, disappearance of CO is therefore not accompanied by large residual oxygen: the available oxygen is consumed while carbon is transferred to more fully oxidised products. Oxygen depletion alone is consequently not a measure of incomplete combustion; it must be interpreted together with CO and temperature.

The $\lambda = 0.60$, 90/10 field is not part of this reacting sequence. Its maximum temperature is only 307 K, its CO-rich area is zero, and almost the entire plane contains more than 1 vol.% oxygen. The low CO concentration therefore indicates lack of ignition or extinction in the steady numerical solution, not efficient CO oxidation. This case should be reported as a cold solution branch and excluded from rankings of combustion performance unless a cold state was intentionally sought. Its residual history, inlet mass flows, initialisation, and ignition procedure should be checked before the result is used to define an operating limit.

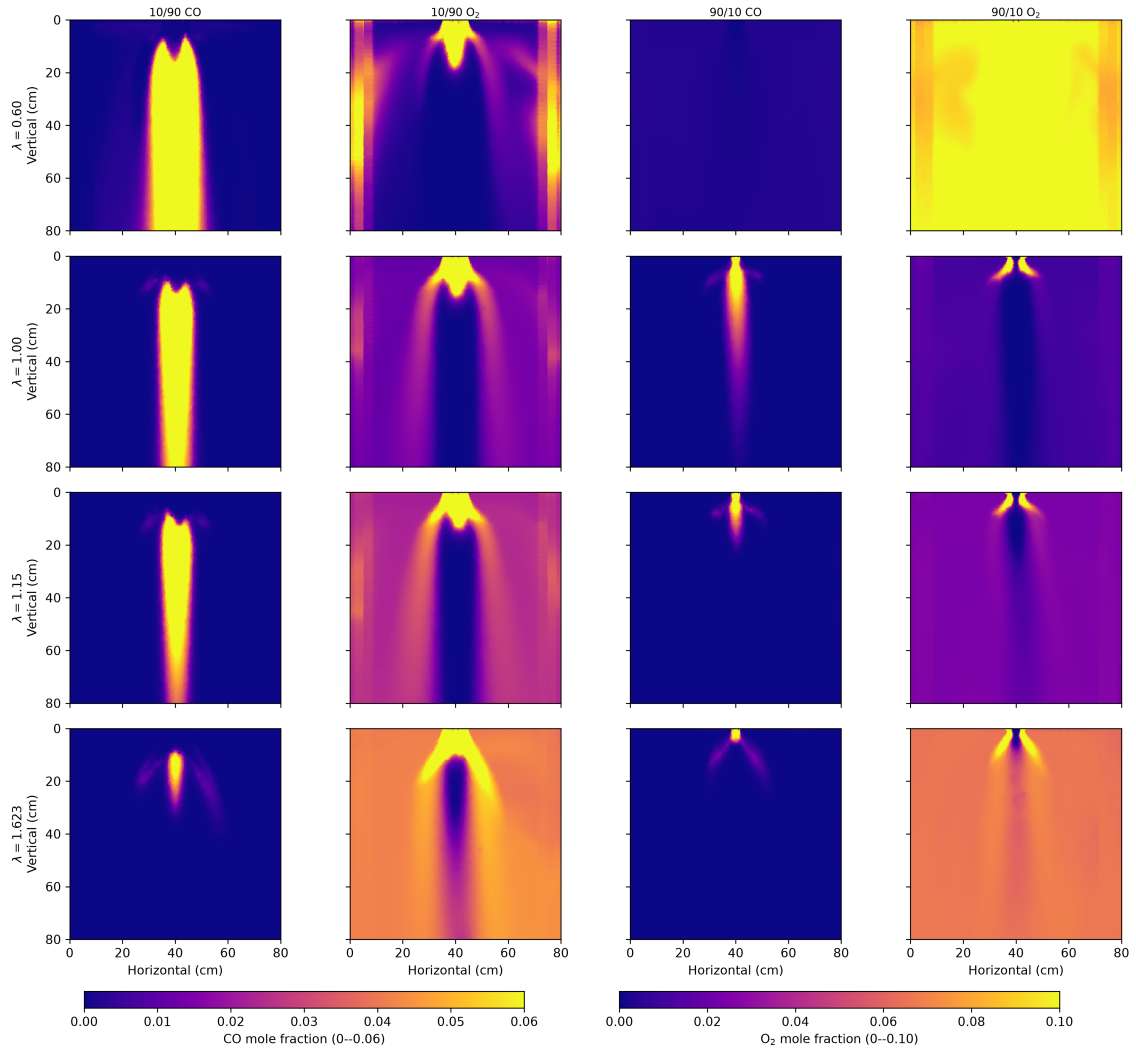


Figure 4.17: CO and oxygen contours for the extreme air distributions across the four excess-air ratios. Common species scales are used in every row.

4.3.3 Intermediate distributions

The 25/75 sequence in Figure 4.18 closely follows the 10/90 and 41.15/58.85 secondary-dominant cases. CO above 1 vol.% occupies 26.59, 16.98, 13.75, and 2.67% of the plane as λ increases from 0.60 to 1.00, 1.15, and 1.623. The corresponding oxygen-depleted fractions are 50.47, 16.50, 13.47, and 2.34%. Thus, for all three cases in which the secondary passage carries most of the air, raising λ monotonically reduces both the size of the oxygen-poor core and the persistence of CO. The field topology remains similar while its axial and radial dimensions contract.

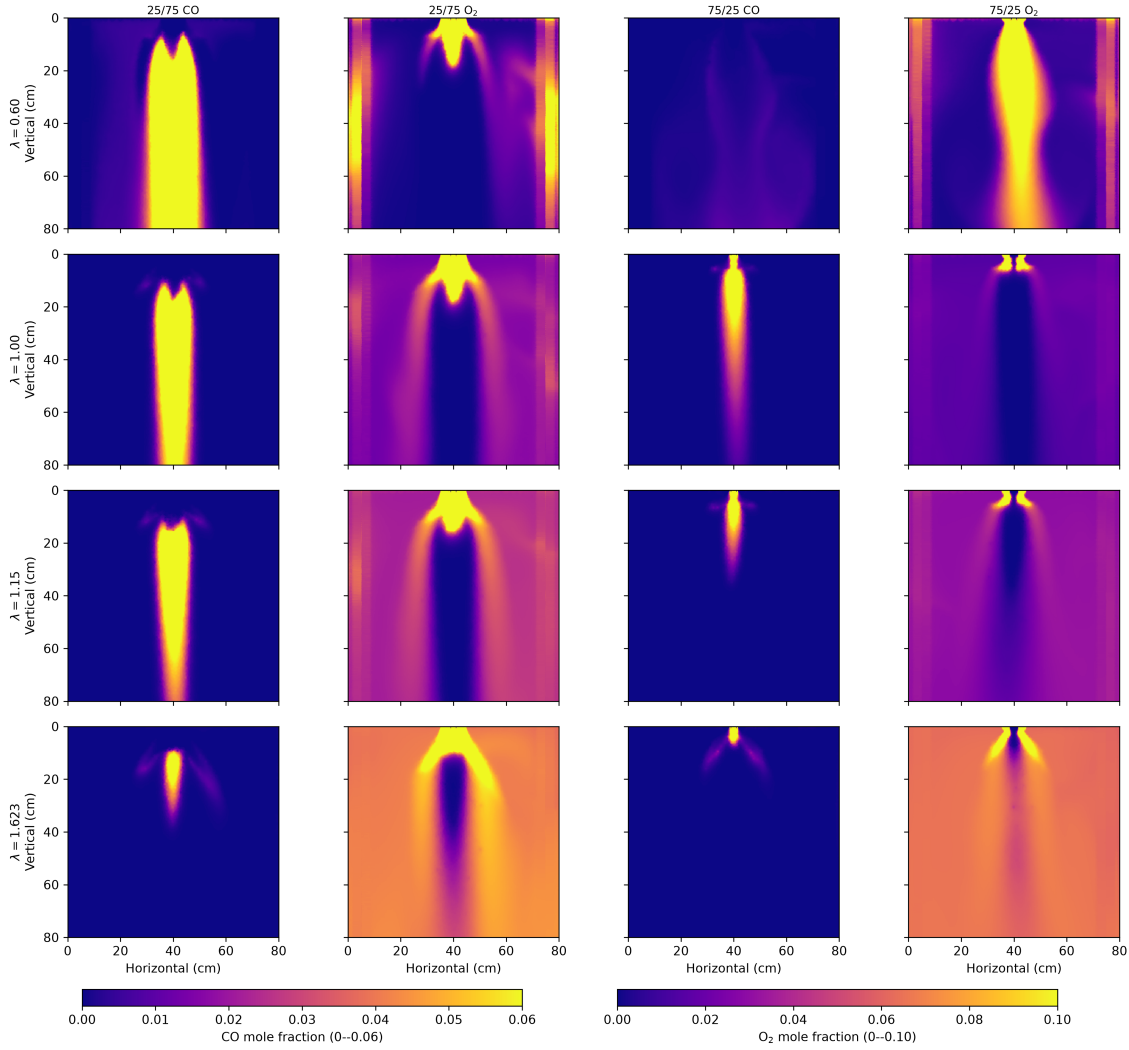


Figure 4.18: CO and oxygen contours for the intermediate air distributions across the four excess-air ratios. Common species scales are used in every row.

The 75/25 result behaves continuously between $\lambda = 1.00$, 1.15, and 1.623: the CO-rich area decreases from 10.02 to 2.78 and 0.83%, and the CO maximum moves progressively closer to the burner. The $\lambda = 0.60$ case does not continue this sequence. Although its CO-rich area is only 0.04%, its maximum temperature is 857 K, compared with approximately 1926–1947 K for the reacting secondary-dominant cases at the same excess-air ratio. Its oxygen field also contains a central oxygen-rich plume rather than the oxygen-depleted reacting core seen in the other rich cases. This combination indicates a weakly reacting or partially extinguished numerical state. As for the cold 90/10 case, the small CO value must not be interpreted as complete combustion.

4.3.4 Axial and M2–M5 concentration profiles

The axial profiles at horizontal positions of 30, 35, and 40 cm and the radial profiles at M2–M5 provide a line-based check of the contour interpretation. The 35 cm axial

4. Results

line is shown in Figure 4.19 because it passes through the annular reacting region. The four excess-air-ratio curves are superimposed in the first two panels so that their ordering and the movement of the CO peak can be compared directly. The 30 and 40 cm lines were also inspected when establishing the trends described below. The radial stations are located at 20, 40, 58, and 80 cm downstream of the burner exit. All curves in this cross-ratio comparison are CFD results; no experimental markers or experimental standard-deviation data are included.

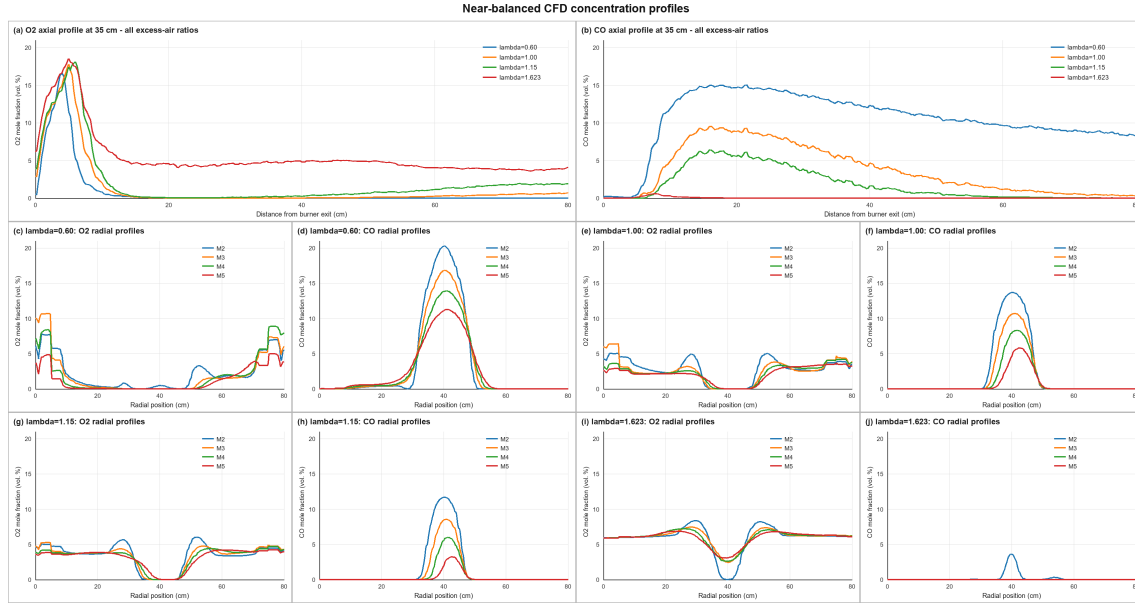


Figure 4.19: CFD-only oxygen and CO profiles for the 41.15/58.85 air split. Panels (a) and (b) superimpose the four excess-air ratios on the axial line at the 35 cm horizontal position. Panels (c)–(j) show the corresponding radial M2–M5 profiles for each ratio. Common 0–20 vol.% ordinate ticks are retained to make the change in concentration magnitude visible.

The combined axial panels show that, for the 41.15/58.85 split, CO is systematically replaced by residual oxygen as excess air is increased. The line-mean CO concentration decreases from 10.58 vol.% at $\lambda = 0.60$ to 3.72, 1.84, and 0.040 vol.% at $\lambda = 1.00$, 1.15, and 1.623, respectively. At the same time, the mean oxygen concentration increases from 0.88 to 1.41, 2.11, and 5.56 vol.%. The CO maximum decreases from 15.06 to 9.55, 6.44, and 0.61 vol.%, and its location moves from 21.5 cm at $\lambda = 0.60$ to 7.5 cm at $\lambda = 1.623$. Thus, added air affects both concentration and flame length: the CO-rich region becomes weaker and its characteristic axial distance contracts towards the burner.

The radial profiles give the same ordering. At M2, the maximum CO concentration for 41.15/58.85 decreases from 20.29 vol.% at $\lambda = 0.60$ to 13.69, 11.72, and 3.64 vol.%. At M5, the corresponding maxima are 11.28, 5.83, 3.24, and approximately 0.0014 vol.%. The mean M5 oxygen concentration simultaneously increases from 1.20 to 2.11, 3.11, and 5.91 vol.%. The early CO profiles are centred close to the furnace centreline at a radial position of 40 cm and are approximately symmetric. Their reduction from M2 to M5 is therefore a real downstream change rather than

the result of plotting only one side of the furnace. Small left–right differences at the later stations are consistent with the imposed three-dimensional air distribution and obstruction by the cooling rods.

The full set of air-split profiles shows that peak concentration alone is not a sufficient performance measure. At $\lambda = 1.00$, 1.15, and 1.623, CO is largest at M2 and generally decays at each downstream station. Once the primary stream carries most of the air, the M5 CO concentration approaches zero and the axial CO maximum moves closer to the burner. Among the secondary-dominant cases, the exact M2 peak is not strictly monotonic with air split because it depends on where a narrow reaction sheet intersects the line. The downstream persistence, profile mean, and CO-rich plane area nevertheless all contract with increasing excess air. The 30 cm profiles sample the outer reaction layer and the 40 cm profiles sample the centreline; together they show that this contraction is not confined to a single axial cut.

The rich $\lambda = 0.60$ profiles in Figure 4.20 require separate attention. For 58.85/41.15, the 35 cm line contains a mean of 10.67 vol.% CO, while the mean M5 oxygen concentration is only 0.00047 vol.% and the mean M5 CO concentration remains 5.80 vol.%. This is a strongly reacting but severely oxygen-starved branch. The 75/25 case behaves differently: its mean radial CO concentration increases from 0.079 vol.% at M2 to 0.465 vol.% at M5, while the oxygen field contains a broad central maximum. The downstream increase in CO is inconsistent with the normal oxidation sequence and supports the classification of this case as weakly reacting or partially extinguished. In the 90/10 case, the mean oxygen concentration on the 35 cm line is 12.63 vol.%, whereas the mean CO concentration is only 0.152 vol.%. In combination with its 307 K maximum temperature, this high-oxygen/low-CO state identifies a cold solution rather than efficient combustion.

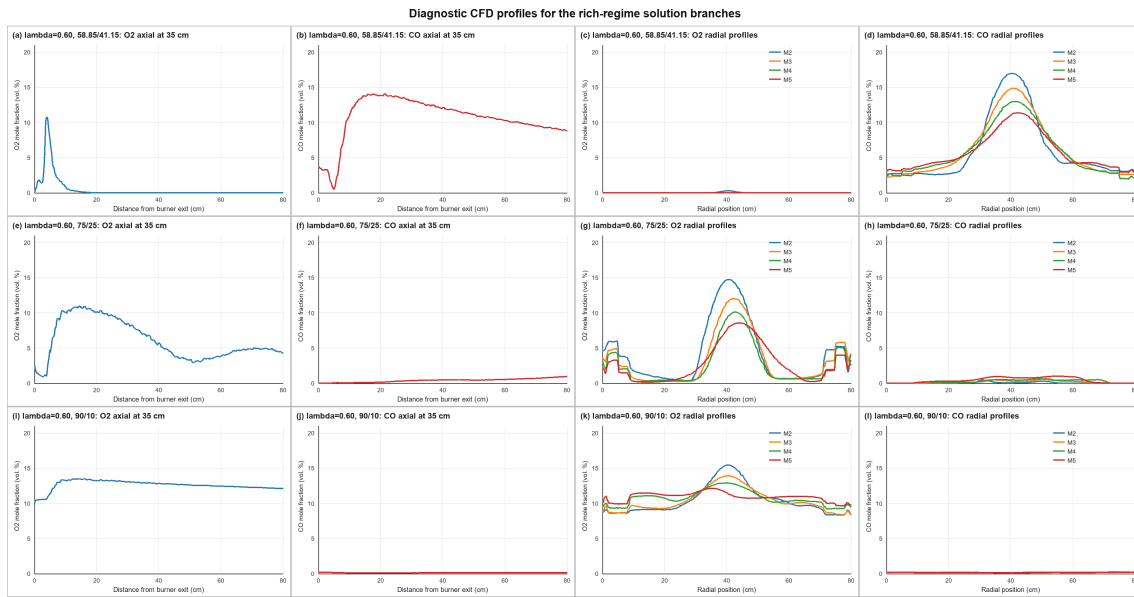


Figure 4.20: CFD-only axial and M2–M5 radial profiles for the three primary-dominant solution branches at $\lambda = 0.60$. The common scales distinguish the reacting oxygen-starved 58.85/41.15 case, the weak 75/25 case, and the cold 90/10 case.

4.3.5 Synthetic infrared flame-image comparison

Figure 4.21 compares three diagnostically useful air splits at all four excess-air ratios. The 10/90 sequence represents a secondary-dominant distribution that maintains a reacting solution throughout the matrix, 41.15/58.85 provides the near-balanced reference, and 90/10 exposes the primary-dominant cold branch at $\lambda = 0.60$. The synthetic images were generated from the saved Fluent fluid and wall exports with the same ray-tracing code and camera geometry. The dark vertical bands are cooling-rod shadows. Every panel uses the common 0–15,000 $\text{W m}^{-2} \text{sr}^{-1}$ colour scale; flame shape, continuity, axial extent, and radiance magnitude can therefore be compared directly.

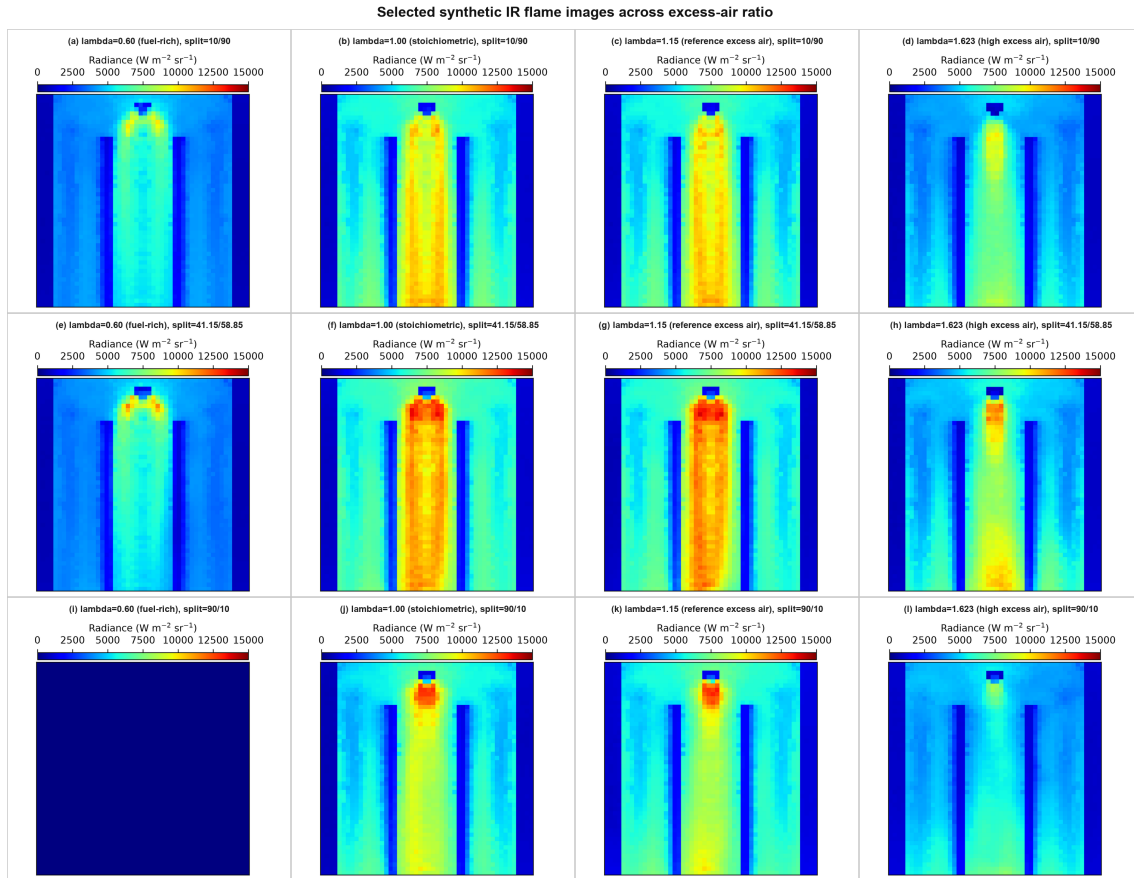


Figure 4.21: Selected synthetic infrared flame images at $\lambda = 0.60, 1.00, 1.15$, and 1.623 . Rows show primary/secondary air splits of 10/90, 41.15/58.85, and 90/10, while columns compare excess-air ratio at a fixed split. Every panel uses the common 0–15,000 $\text{W m}^{-2} \text{sr}^{-1}$ radiance scale.

4.3.5.1 Direct comparison of $\lambda = 0.60$ and 1.15 for all air splits

Under the definition in Equation 3.13, $\lambda = 0.60$ is a fuel-rich condition, not a lean condition, because the supplied air is only 60% of the stoichiometric requirement. Figures 4.22 and 4.23 compare it directly with the reference $\lambda = 1.15$ condition for every air split. Each image uses the common 0–15,000 $\text{W m}^{-2} \text{sr}^{-1}$ radiance range,

so identical colours represent identical intensity.

For 10/90, reducing λ from 1.15 to 0.60 replaces the long, continuous high-radiance column with a compact twin-lobed source at the burner and a much more diffuse central field. The 25/75 pair shows the same change: the reference flame remains long and connected, whereas the rich solution is dominated by two near-burner lobes. In both secondary-dominant cases, insufficient global oxygen limits conversion to hot radiating products even though the species fields retain a CO-rich reacting region. At 41.15/58.85, the $\lambda = 1.15$ image contains an elongated but narrower central column; at $\lambda = 0.60$, emission is again concentrated in the twin near-burner lobes and the downstream column loses definition. Reversing the near-balanced split to 58.85/41.15 contracts the $\lambda = 1.15$ flame towards the burner, but it still retains a coherent reacting source. Its $\lambda = 0.60$ counterpart is weaker and more diffuse downstream, showing that the rich flame is more sensitive to redistribution of inlet momentum.

The 75/25 pair marks a change of solution branch. At $\lambda = 1.15$, the image has a compact high-radiance base with a weak axial continuation. At $\lambda = 0.60$, the field becomes broad and weak on the common scale, without the coherent central flame topology found in the secondary-dominant rich cases. The 90/10 contrast is stronger still: the $\lambda = 1.15$ case retains a localised reacting source with radiance in the thousands, whereas the $\lambda = 0.60$ radiance is only about $1.5\text{--}2.2 \text{ W m}^{-2} \text{ sr}^{-1}$ and no flame column is visible. Together with its approximately 307 K maximum temperature, the latter is a cold numerical solution rather than a low-CO, high-efficiency flame.

The convergence balances support this distinction but do not justify treating all rich images as equivalent. For the checked 25/75 case at $\lambda = 1.15$, the net total heat-transfer rate was -767.7 W , the mass imbalance was 0.000177% , and the heat-balance error was 0.907% . For $\lambda = 0.60$, 25/75, the residuals were stable and the mass imbalance was only $2.11 \times 10^{-7}\%$, but the net total heat-transfer rate was $+2822.7 \text{ W}$, giving a 5.521% heat-balance error. This is slightly above the adopted 5% limit. The rich 25/75 result, and especially the cold primary-dominant branch, must therefore be interpreted qualitatively; residual stability alone is not evidence of a quantitatively converged flame.

The full balance audit in Appendix D.1 reinforces this interpretation. The master 41.15/58.85 case at $\lambda = 1.15$ closes mass to 0.0000913% and energy to 1.663% , with 84.151 kW released by reaction and 85.574 kW accounted for at the outlet and cooled boundaries. All six $\lambda = 1.00$, all six $\lambda = 1.15$, and all six $\lambda = 1.623$ air-split cases satisfy the 5% energy criterion. By contrast, four of the six $\lambda = 0.60$ reacting cases exceed it: 10/90, 25/75, 41.15/58.85, and 75/25 have errors of 8.59 , 5.52 , 5.53 , and 63.40% , while the cold 90/10 solution gives essentially zero reaction heat and a nominal 100% imbalance. These cases are therefore used only to identify branch changes and qualitative image behaviour. The audit also identified a boundary-condition inconsistency in the $\lambda = 1.00$, 58/41 file: its total inlet flow is $0.033508 \text{ kg s}^{-1}$ rather than the $0.028730 \text{ kg s}^{-1}$ used by the other five splits at that ratio. Although its mass and energy balances close, it is not a controlled constant-total-flow comparison and is interpreted with this qualification.

At $\lambda = 1.00$, the 10/90 and 41.15/58.85 cases form continuous central emission

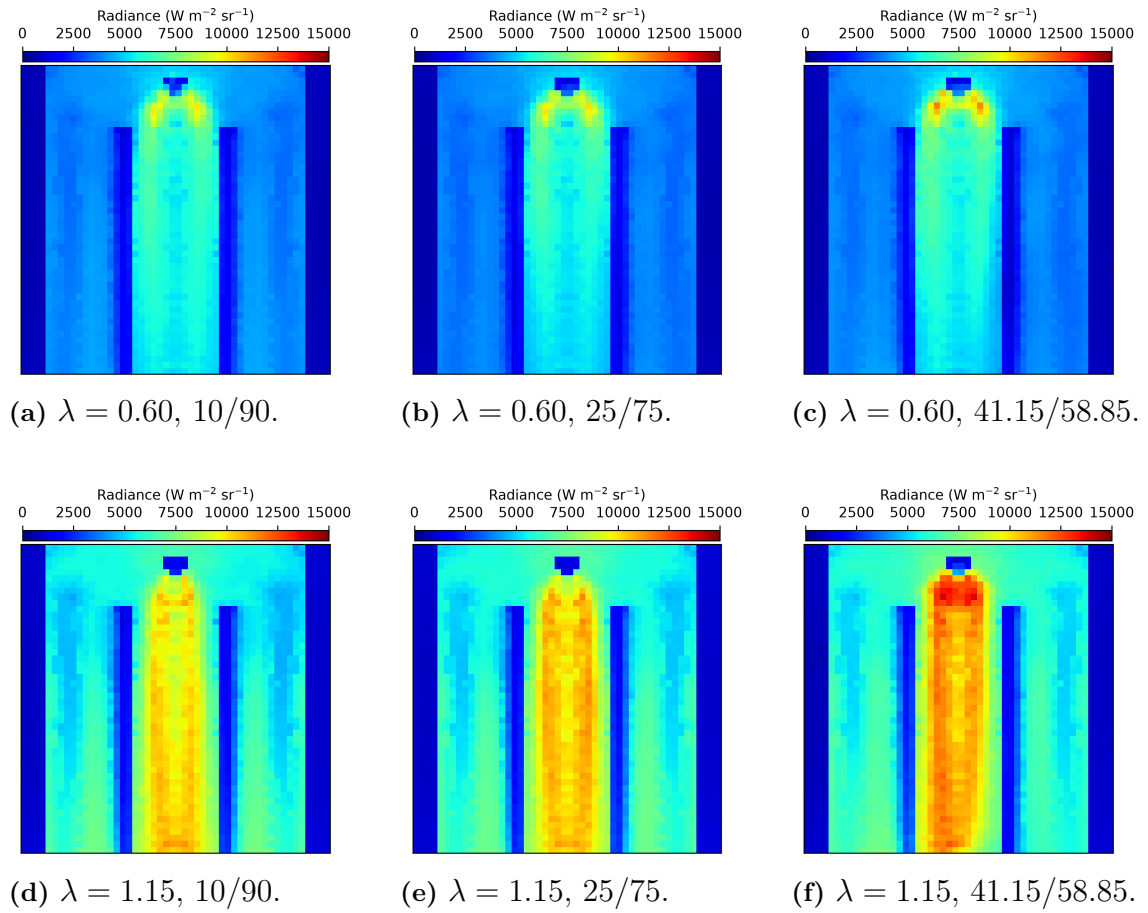


Figure 4.22: Synthetic infrared comparison of $\lambda = 0.60$ and 1.15 for the secondary-dominant and reference air splits, using a common $0\text{--}15,000 \text{ W m}^{-2} \text{sr}^{-1}$ colour scale.

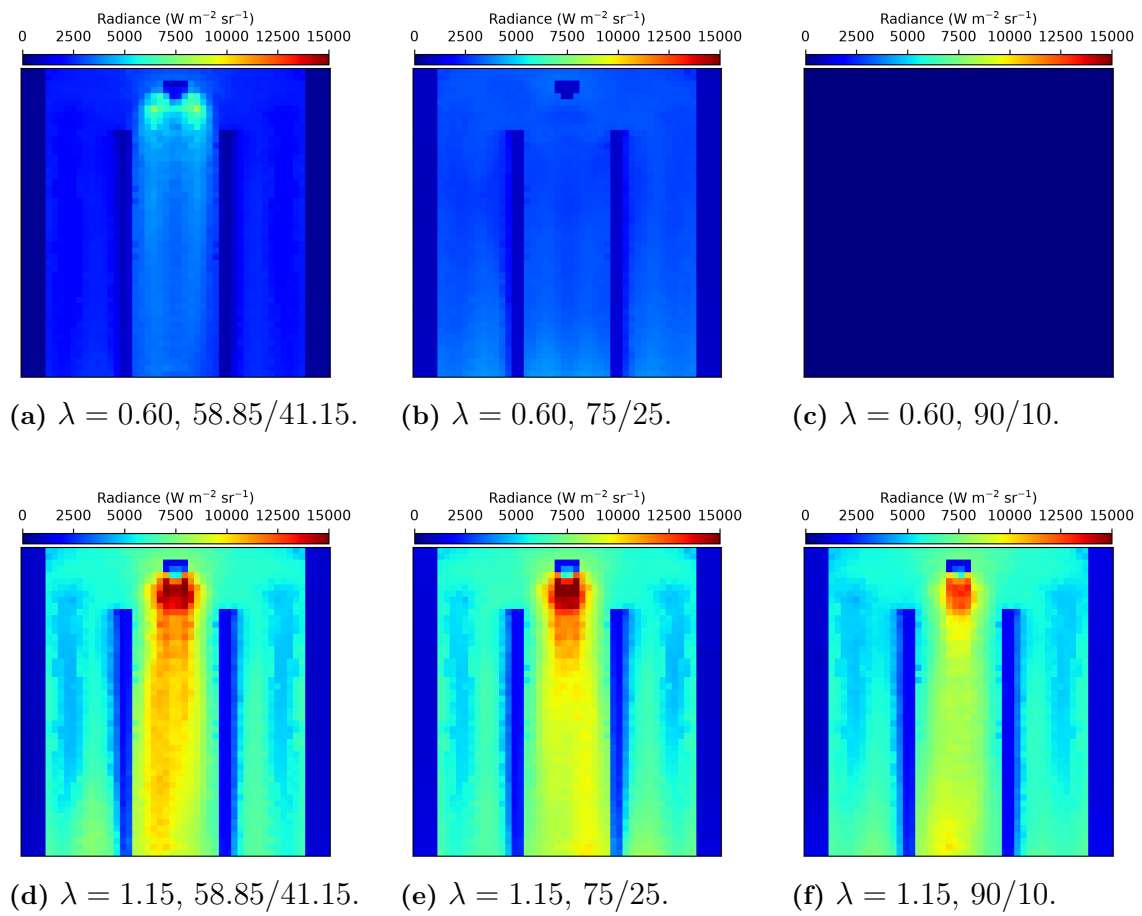


Figure 4.23: Synthetic infrared comparison of $\lambda = 0.60$ and 1.15 for the primary-dominant air splits, using a common $0\text{--}15,000 \text{ W m}^{-2} \text{sr}^{-1}$ colour scale.

columns extending far downstream of the burner. The secondary- dominant 10/90 column is broader and more persistent, whereas increasing the primary fraction to 41.15/58.85 narrows the emitting core. The 90/10 flame is shorter and its strongest feature remains closer to the burner. At the stoichiometric global condition, redistribution of the same total air flow therefore changes the residence and mixing path sufficiently to control flame length even though all three selected cases remain reacting.

At the reference condition $\lambda = 1.15$, the 10/90 flame retains the longest continuous high-emission column, and the 41.15/58.85 flame remains elongated but narrower. The 90/10 image is again dominated by a compact near-burner source with a weaker downstream path. This ordering agrees with the oxygen and CO contours: a high secondary-air fraction delays inward oxidiser transport and sustains the reacting product column, while a high primary-air fraction promotes earlier mixing and spatial contraction.

At $\lambda = 1.623$, a compact near-burner source remains visible, but the continuous high-emission column characteristic of $\lambda = 1.00$ and 1.15 is replaced by a more diffuse and partly disconnected downstream field. This occurs for both the 10/90 and 41.15/58.85 sequences and is strongest for the 90/10 split. The corresponding concentration fields contain more residual oxygen and substantially less persistent CO. The flame images therefore support a combined chemical and thermal interpretation: high excess air shortens the locally rich reaction zone and dilutes the hot radiating products, rather than merely shifting an otherwise unchanged flame.

The 41.15/58.85 row gives the clearest cross-ratio comparison. Its flame is compact under the globally rich $\lambda = 0.60$ condition, becomes long and continuous at $\lambda = 1.00$ and 1.15 , and contracts into a short source with diffuse downstream emission at $\lambda = 1.623$. Flame extent is therefore non-monotonic across the complete excess-air-ratio range: too little air limits hot-product formation, while very high excess air contracts and dilutes the reaction zone. The longest synthetic infrared column occurs between these two limits rather than at either endpoint.

4.4 Effect of propane mass-flow rate

The propane-flow series isolates a different parameter from the preceding excess-air study. The excess-air ratio was held at $\lambda = 1.15$, the primary/secondary split was retained at 41.15/58.85, and the total air flow was increased in direct proportion to the propane flow according to Table 3.6. Consequently, the global air-to-fuel ratio was unchanged, whereas the total inlet momentum, thermal input, turbulent mixing rate, and convective residence time were allowed to change. The four CFD cases used propane flows of 1.0, 1.5, 2.0, and 3.0 g s^{-1} . The experimental symbols in the figures are the fixed measurements at the 1.73 g s^{-1} reference condition; they are a matched comparison only for the reference calculation and are not measurements of the four fuel-flow cases. That reference is the experimental condition shown in Figure 4.1; the other fuel flows are numerical departures from it rather than additional validations. Figure 4.24 shows that the oxygen and CO fields do not scale geometrically with firing rate even though λ is fixed. At 1.0 g s^{-1} , the oxygen-depleted core is surrounded by a comparatively oxygen-rich outer field. Increasing the flow to 1.5 and

2.0 g s^{-1} reduces this outer residual oxygen and retains a long, nearly centred oxygen-poor core. These two cases bracket the baseline flow of 1.73 g s^{-1} and most closely preserve its contour topology. The 3.0 g s^{-1} case is qualitatively different: the high-oxygen near-burner region penetrates farther into the furnace, while the downstream oxygen-depleted region becomes narrower and displaced from the symmetry line. The CO contours provide the complementary interpretation. The 1.0 and 1.5 g s^{-1} cases contain a broad CO-rich column that persists well downstream, and the 2.0 g s^{-1} result is similar but narrower. At 3.0 g s^{-1} , the CO-rich region contracts strongly in the radial direction and its maximum on the 35 cm line occurs farther downstream. This does not mean that the high-flow case produces less CO everywhere. Rather, the simultaneous increase in inlet velocity transports the mixing and oxidation sequence downstream and changes where a fixed line or probe row intersects the reaction zone.

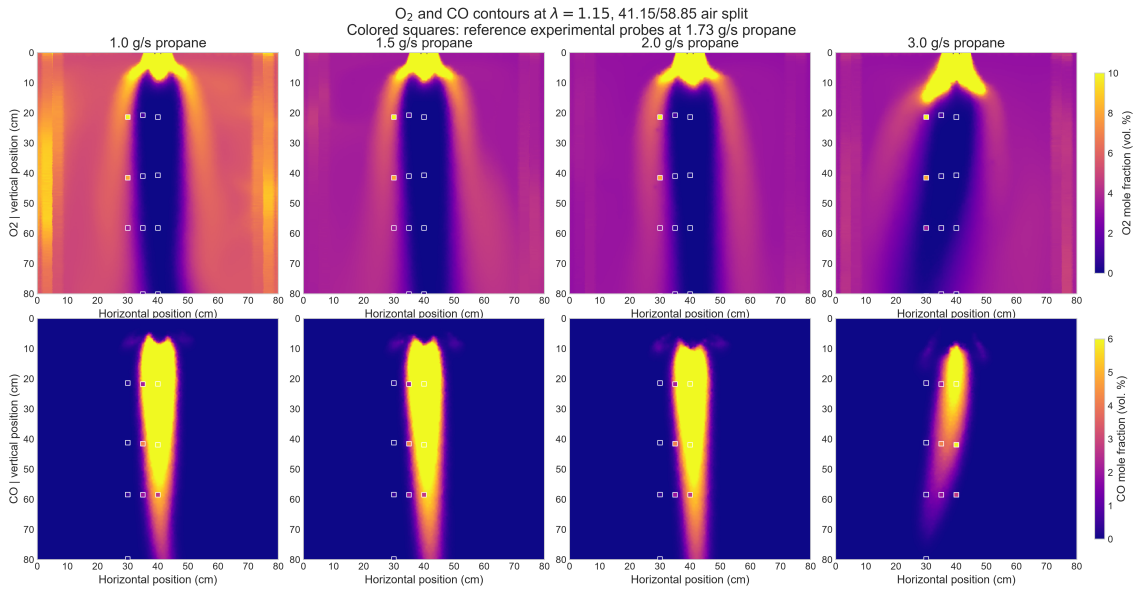
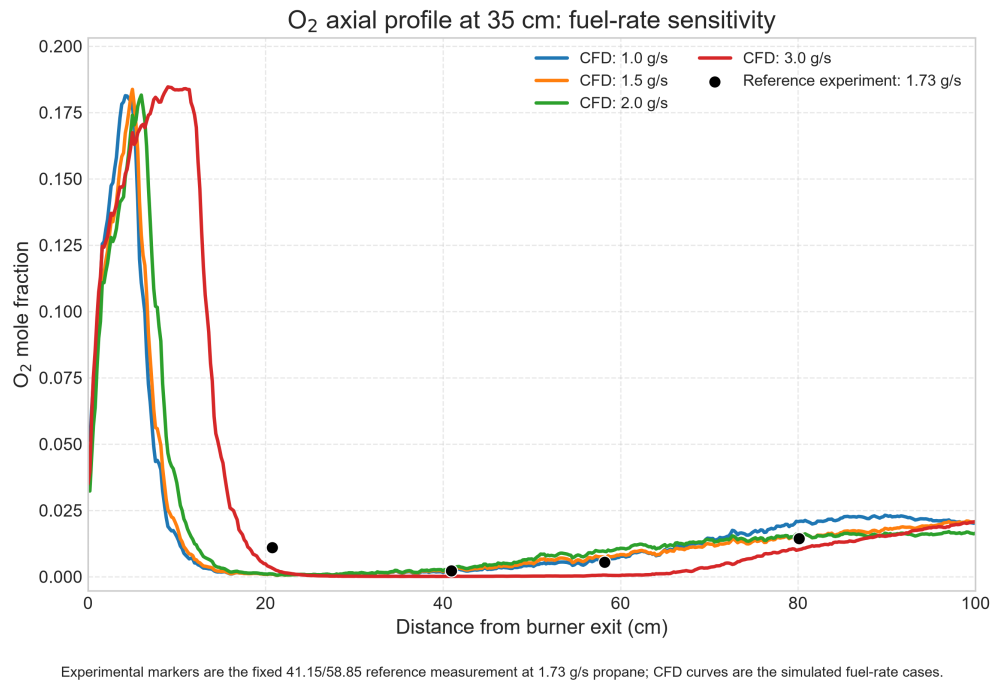


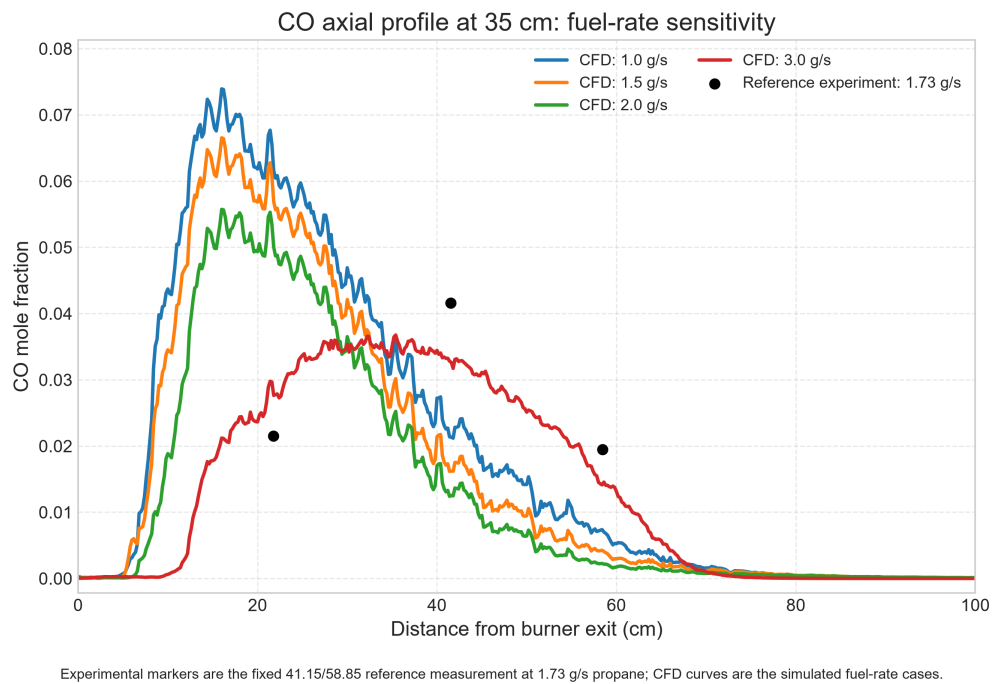
Figure 4.24: CFD oxygen and CO contours for the propane-flow series at $\lambda = 1.15$ and the 41.15/58.85 air split. Common ranges of 0–10 vol.% oxygen and 0–6 vol.% CO are used. Coloured squares show the fixed 1.73 g s^{-1} reference measurements and are not separate experiments for each simulated flow.

The axial profiles in Figure 4.25 quantify the contour changes on the 35 cm horizontal line. The oxygen maximum remains within the narrow range 18.13–18.46 vol.% for all four cases, but its axial extent changes markedly. In the 1.0 – 2.0 g s^{-1} cases the high-oxygen inlet feature collapses within approximately the first 15 cm. At 3.0 g s^{-1} , it persists farther downstream and the subsequent oxygen-poor interval extends to approximately 60 cm before recovery begins. The line-mean oxygen concentrations are 1.86, 1.77, 1.94, and 2.66 vol.% for increasing fuel flow. Thus, the high-flow increase in the oxygen mean is caused principally by the longer near-burner oxygen feature; it does not represent uniformly oxygen-rich conditions downstream.

The CO line contains both a magnitude change and a location change. Its maximum decreases from 7.39 to 6.65 and 5.57 vol.% as the propane flow increases from 1.0 to 1.5 and 2.0 g s^{-1} ; all three maxima occur at approximately 16 cm. The reference



(a) Oxygen.



(b) Carbon monoxide.

Figure 4.25: Axial CFD profiles on the 35 cm horizontal line for the propane-flow series. Black symbols are the fixed 1.73 g s^{-1} reference experiment. Oxygen and CO are given equal space so that changes in extent and peak location remain visible for both species.

$\lambda = 1.15$ CFD result at 1.73 g s^{-1} lies between these cases, with a maximum of 6.44 vol.% and a line mean of 1.84 vol.%. At 3.0 g s^{-1} , the maximum is lower at 3.68 vol.%, but it moves to 35.4 cm and the CO profile becomes a broad plateau. Its line mean is 1.38 vol.%, close to the 1.33 vol.% obtained at 2.0 g s^{-1} . Peak CO alone would therefore give a misleading ranking: the 3.0 g s^{-1} case has a smaller local maximum but a delayed and spatially redistributed CO field.

The radial oxygen profiles in Figure 4.26 reinforce this distinction. At M2, the line-mean oxygen concentration is 5.11 vol.% at 1.0 g s^{-1} , compared with 3.30, 3.06, and 3.05 vol.% at 1.5, 2.0, and 3.0 g s^{-1} . The 1.0 g s^{-1} case therefore leaves substantially more oxygen in the outer flow while maintaining an oxygen-depleted centre. At 1.5 and 2.0 g s^{-1} , the central depleted region and its two shoulders remain approximately symmetric from M2 to M5 and most closely resemble the reference topology. At 3.0 g s^{-1} , the minimum shifts progressively to the left at M3–M5, showing that the high-throughput flame and mixing layer no longer intersect the measurement planes symmetrically. The remaining mismatch with the reference shoulder values, particularly at M2 and M3, also shows that bracketing the reference fuel flow does not remove the model discrepancy in the steep reaction-sheet region.

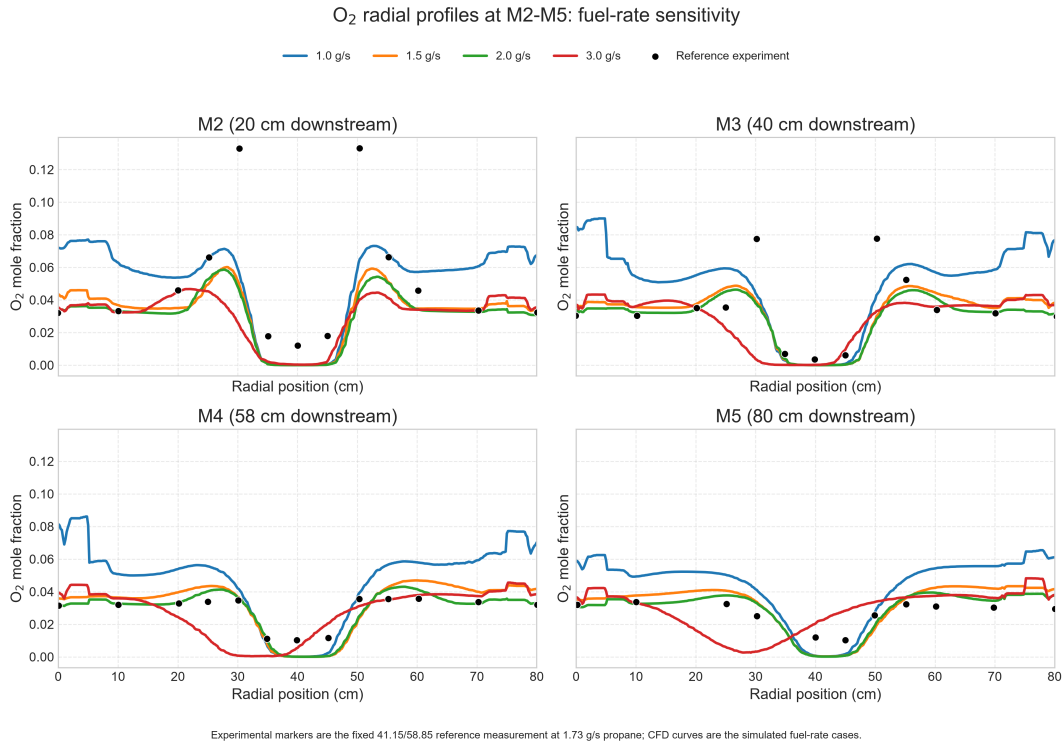


Figure 4.26: Radial oxygen profiles at M2–M5 for the propane-flow series. Black symbols are the fixed 1.73 g s^{-1} experiment. The common ordinate exposes the elevated outer oxygen at 1.0 g s^{-1} and the displaced depleted core at 3.0 g s^{-1} .

The radial CO profiles in Figure 4.27 show a more pronounced fuel-flow sensitivity. At M2, the maximum decreases from 12.28 to 11.72, 10.80, and 6.89 vol.% as flow increases. The 1.0 – 2.0 g s^{-1} profiles remain centred at approximately 40 cm and retain downstream maxima of 2.23–2.76 vol.% at M5. In contrast, the 3.0 g s^{-1} peak moves from 39.6 cm at M2 to 37.8 cm at M3 and 33.4 cm at M4, while its M5

maximum falls to approximately 0.013 vol.%. The same case that gives a delayed broad CO distribution on the 35 cm axial line therefore gives almost no CO on the M5 radial line. Taken together, these cuts indicate downstream displacement followed by rapid consumption, rather than a uniform reduction throughout the furnace.

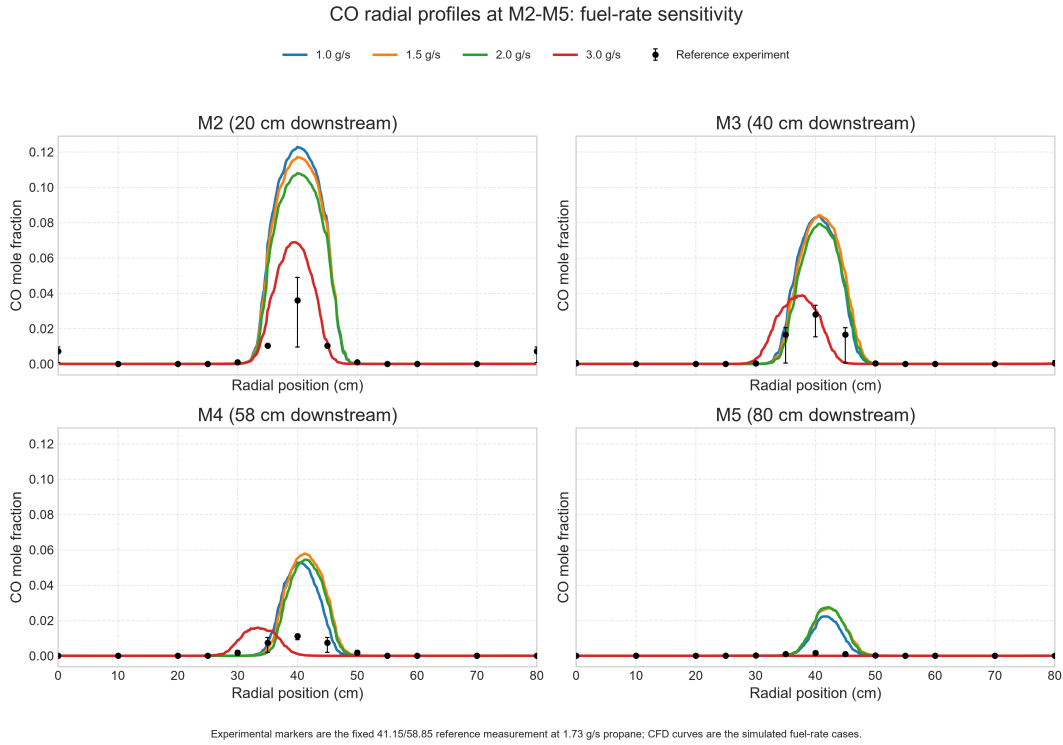


Figure 4.27: Radial CO profiles at M2–M5 for the propane-flow series. Error bars and black symbols belong to the fixed 1.73 g s^{-1} reference experiment. The high-flow case has lower local peaks but also a shifted reaction path.

The physical origin of these changes is the loss of dynamic similarity when the firing rate is varied. Maintaining λ fixes the overall air-to-fuel mass ratio, but it does not fix inlet velocity, Reynolds number, turbulent strain, wall heat loss per unit fuel input, or residence time. The 1.5 and 2.0 g s^{-1} cases surround the 1.73 g s^{-1} baseline and retain a similar balance between convection and radial entrainment. The 1.0 g s^{-1} case shows weaker cross-stream consumption, expressed as higher outer oxygen together with a strong central CO peak. At 3.0 g s^{-1} , greater inlet momentum carries the oxygen-rich and CO-forming zones farther downstream, while stronger turbulent mixing and the higher thermal input subsequently accelerate CO removal before M5. This interpretation is consistent with both species and should not be inferred from either the oxygen or CO peak in isolation.

4.4.1 Synthetic infrared response to firing rate

Figure 4.28 compares the four generated flame images with the existing 1.73 g s^{-1} baseline. The same ray-tracing model, spectral range, camera geometry, and cooling-

rod representation were used in every case. All panels use the common $0\text{--}15,000\text{ W m}^{-2}\text{ sr}^{-1}$ radiance scale, so identical colours represent identical intensity.

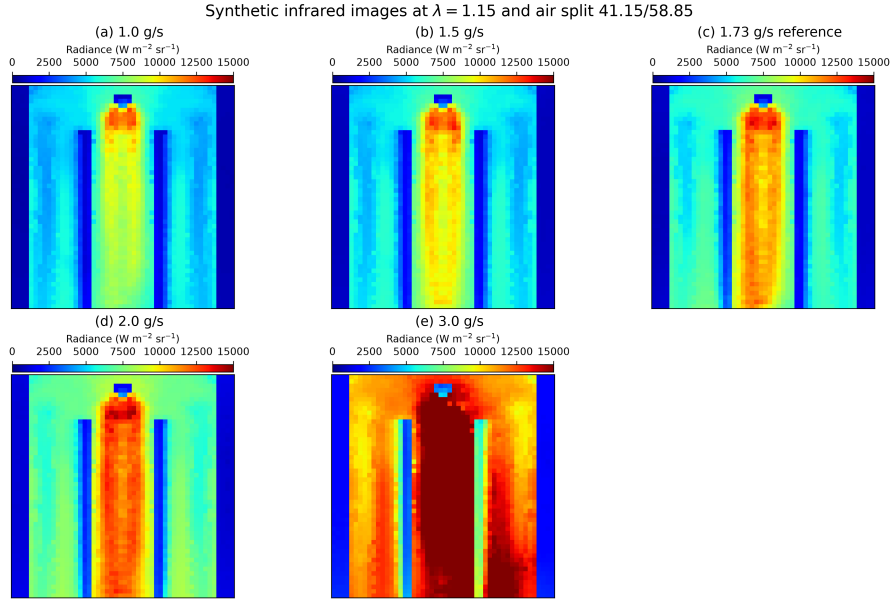


Figure 4.28: Synthetic infrared images for the propane-flow series and the 1.73 g s^{-1} baseline at $\lambda = 1.15$ and the $41.15/58.85$ air split. Dark vertical bands are cooling-rod shadows. Colour bars report radiance on the common $0\text{--}15,000\text{ W m}^{-2}\text{ sr}^{-1}$ scale.

Here, 1.15 denotes the fixed excess-air ratio; the reference fuel flow is 1.73 g s^{-1} . Reducing the propane flow from the 1.73 g s^{-1} reference to 1.0 g s^{-1} preserves a centred, continuous emitting column, but the column becomes narrower and its radiance is the lowest of the sequence on the common scale. The compact high-emission region remains attached to the burner, so the lower firing rate does not produce the displacement seen at 3.0 g s^{-1} . Instead, the smaller fuel and proportional air flows reduce the thermal input and the amount of hot radiating product along the camera line of sight. The result is a weaker and more confined image than the nominal 1.73 g s^{-1} flame, consistent with the higher outer oxygen and strong central CO peak predicted at 1.0 g s^{-1} .

The increase from 1.5 to 2.0 g s^{-1} , with the 1.73 g s^{-1} reference between them, is gradual rather than a change of flame regime. All three images retain a continuous central column, a compact near-burner maximum, and comparable left–right extent between the cooling rods. From 1.5 through 1.73 to 2.0 g s^{-1} , the high-emission column becomes more uniformly intense and the surrounding furnace field becomes stronger, while the flame axis remains almost unchanged. Since λ and the air split are fixed, this increase is not caused by a richer global mixture. It follows from the higher firing rate and proportional increase in total throughflow, which increase the hot-product inventory and radiative path contribution while retaining a similar balance between convection and radial mixing. This morphological continuity agrees with the oxygen and CO contours and confirms that the 1.5 and 2.0 g s^{-1} calculations bracket the baseline response.

The 3.0 g s^{-1} image is the clear exception: parts of it exceed the $15,000 \text{ W m}^{-2} \text{ sr}^{-1}$ display limit and therefore saturate, while the high-emission column broadens and bends to one side. The higher firing rate increases the hot-product inventory and the radiating CO_2 and H_2O path contribution. Its asymmetry also agrees with the displaced M3–M5 oxygen minimum and CO peak, so it is a flow-field feature amplified by the camera line of sight rather than a colour-scale artefact. Relative to 1.73 g s^{-1} , the high-flow change is therefore increased intensity together with broadening and displacement of the reacting product column.

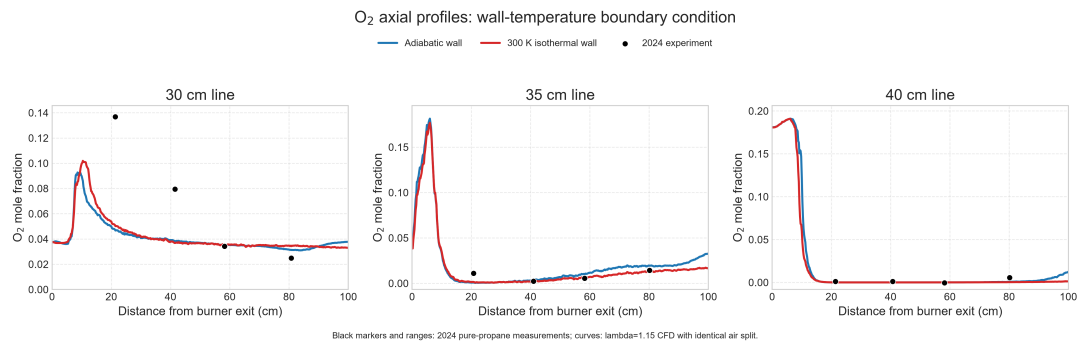
4.5 Effect of the wall-temperature boundary condition

The wall-temperature study isolates the thermal boundary condition while retaining the reference excess-air ratio, $\lambda = 1.15$, the 41.15/58.85 primary/secondary air split, the inlet definitions, and the common mesh. The reference calculation treats the furnace walls as adiabatic, whereas the comparison case fixes them at 300 K. The latter is an intentionally strong heat sink rather than a representation of the measured wall-temperature distribution. Black markers in Figures 4.29 and 4.30 are the pure-propane measurements of Colin et al. [1]; radial bars show the reconstructed minimum-to-maximum ranges. The published experimental contour remains available in Figure 4.1 and is not repeated here.

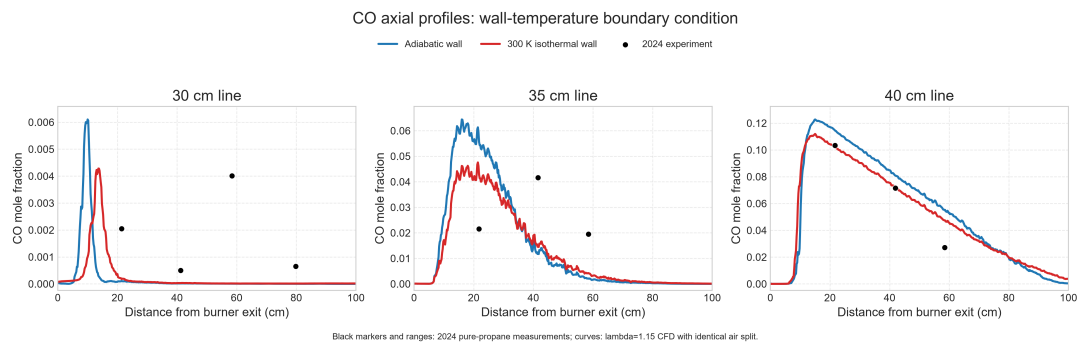
4.5.1 Axial oxygen and CO profiles

Figure 4.29 shows that oxygen is less sensitive to the thermal boundary than CO. On the 30 cm line, the 300 K condition increases the oxygen maximum from 9.27 to 10.19 vol.% and moves it from 8.6 to 10.4 cm downstream. On the 35 and 40 cm lines, the inlet maxima remain close to those of the adiabatic case, but the downstream oxygen recovery is weaker: the line means decrease from 2.15 to 1.76 vol.% and from 2.04 to 1.81 vol.%, respectively. The oxygen-depleted interval is therefore retained under both wall conditions. This indicates that its position is governed primarily by inlet mixing and stoichiometry, while wall cooling modifies the rate at which oxygen reappears outside the principal reaction zone.

The CO response contains both suppression and displacement. At 30 cm, the CO maximum falls from 0.610 to 0.428 vol.% and moves from 10.0 to 13.6 cm. At 35 cm, the maximum decreases from 6.44 to 4.76 vol.% and shifts farther downstream, from 16.0 to 21.4 cm. On the 40 cm line, the maximum remains at approximately 15 cm but decreases from 12.27 to 11.19 vol.%. The cold wall therefore contracts the strongest CO-forming region while delaying the smaller off-centre feature. It does not imply uniformly faster CO oxidation: CO is an intermediate whose local concentration reflects formation, oxidation, convection, and mixing simultaneously. Here the imposed heat loss suppresses and redistributes the high-CO reaction zone. At the experimental points, the 300 K wall improves the CO root-mean-square error on the 35 cm line from 2.84 to 2.20 percentage points and on the 40 cm line from 1.83 to 1.18 percentage points. The oxygen change is mixed: agreement improves



(a) Oxygen.



(b) Carbon monoxide.

Figure 4.29: Axial oxygen and CO mole-fraction profiles on the 30, 35, and 40 cm horizontal lines for the adiabatic and 300 K wall calculations at $\lambda = 1.15$. Black symbols are the 2024 pure-propane measurements. Both species use the same CFD extraction and experimental locations.

on the 35 cm line but changes little or becomes slightly poorer on the 40 cm line. The cold-wall calculation therefore reduces the principal CO overprediction without resolving the oxygen-distribution mismatch. This is important because an apparent improvement in one intermediate species can be caused by compensating thermal error rather than a corrected mixing field.

4.5.2 Radial profiles at M2–M5

The radial profiles in Figure 4.30 reinforce the different sensitivities of the two species. Both wall treatments predict an oxygen-depleted centre at every station. Cooling increases the shoulder maxima moderately, from 5.86 to 6.61 vol.% at M2 and from 4.70 to 5.01 vol.% at M4, but the line means remain within approximately 0.05 percentage points of the adiabatic values. The largest experimental M2 oxygen lobes are still underpredicted, and the root-mean-square error does not improve consistently across M2–M5. Wall heat loss therefore changes the shoulder strength but not the central oxygen-depletion topology that is set by radial entrainment and the air-register flow field.

CO changes systematically. Cooling lowers every calculated maximum: from 11.50 to 10.31 vol.% at M2 and from 8.41 to 7.47 vol.% at M3. Farther downstream, the maximum decreases from 5.98 to 5.07 vol.% at M4 and from 3.23 to 2.46 vol.% at M5. The peak remains close to the furnace centreline, so the downstream ordering is preserved while the amplitude is reduced. Relative to the experimental averages, the radial CO root-mean-square error decreases at every station: from 3.14 to 2.60 percentage points at M2, 1.72 to 1.48 at M3, 1.45 to 1.21 at M4, and 0.78 to 0.62 at M5. Although the 300 K boundary moves the calculation closer to the measurements, the model continues to overpredict the central CO region. The result suggests that heat loss is one contributor to the discrepancy, but not its sole cause.

4.5.3 Synthetic infrared response

The synthetic images in Figure 4.31 show a much larger boundary-condition effect than the species profiles. With adiabatic walls, emission fills most of the camera view and the central high-intensity column remains embedded in a bright furnace background. Fixing the walls at 300 K removes most of this peripheral emission and leaves a narrow, centred radiating column whose strongest region is attached to the burner. On the common scale, the strong reduction in both background and central radiance is directly visible.

The flame-image contraction should not be interpreted as an equivalent shortening of the chemical flame. The camera integrates wall radiation and gas-band emission from hot CO_2 and H_2O along each line of sight, whereas the O_2 and CO plots sample local composition. A 300 K wall simultaneously darkens the background, cools near-wall gas, and alters reaction rates. The comparison therefore demonstrates that a realistic wall thermal model is essential for matching both concentration measurements and optical flame appearance. The 300 K case improves the CO comparison but is too severe to be accepted solely on that basis; measured wall temperatures or a conjugate heat-transfer boundary would be required for quantitative thermal

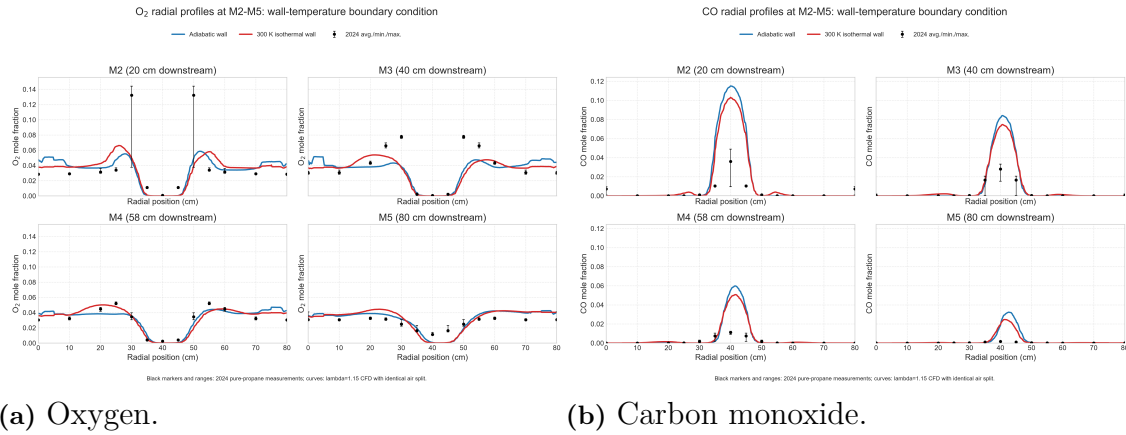


Figure 4.30: Radial oxygen and CO mole-fraction profiles at M2–M5 for the adiabatic and 300 K wall calculations. Black points show the experimental averages, and the vertical bars show the reconstructed minimum-to-maximum ranges from the 2024 pure-propane study.

Synthetic infrared response to the wall-temperature boundary condition

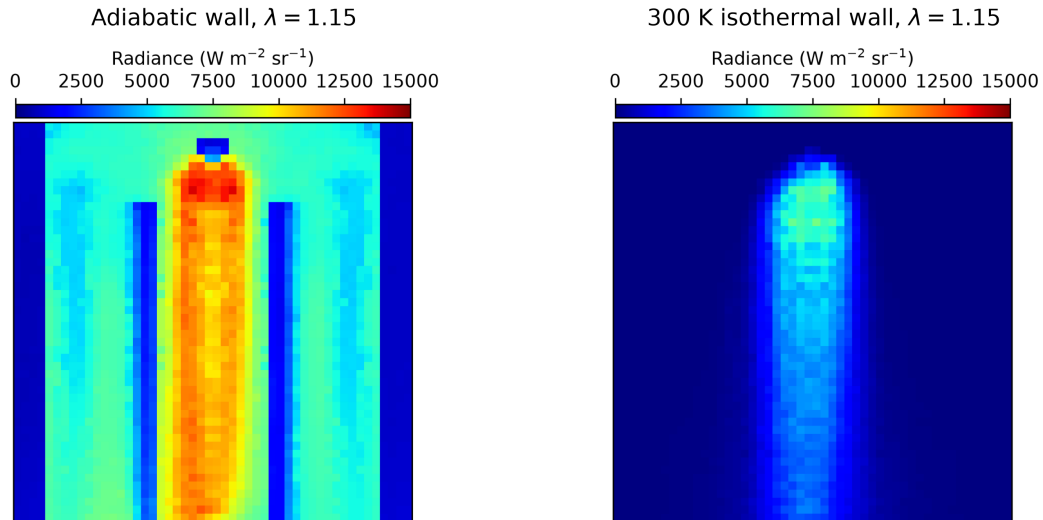


Figure 4.31: Synthetic infrared images for the adiabatic and 300 K wall calculations at $\lambda = 1.15$ and the 41.15/58.85 air split. Colour bars use the common 0–15,000 $\text{W m}^{-2} \text{sr}^{-1}$ radiance range. The large background reduction in the 300 K case reflects both colder wall emission and cooling of the adjacent gas.

validation.

The balance results provide an additional numerical check on this comparison. The 300 K wall case has a mass imbalance of only 0.0000234% and an energy imbalance of 0.297%, so its dark appearance is not a symptom of an unconverged flux balance. In the fuel-flow series, the 1.0, 2.0, and 3.0 g s⁻¹ cases close energy to 3.60, 0.27, and 3.17%, respectively. The 1.5 g s⁻¹ case gives 5.96% and is consequently treated as qualitative where its absolute thermal quantities are discussed.

5

Conclusion

This thesis examined whether simulated changes in combustion state can be distinguished in infrared images. A steady propane–air CFD model of the Chalmers 100 kW unit was coupled to a Statistical Narrow-Band Model and line-of-sight ray tracing. The resulting common-scale images were interpreted together with temperature, O_2 , and CO fields. Comparison with the 2024 pure-propane measurements provided qualitative validation of the principal species topology while also exposing substantial local concentration errors. The CFD therefore supports controlled operating-trend analysis, although it does not reproduce every measured concentration quantitatively.

The main result is that the virtual camera distinguished the stable operating changes. At $\lambda = 1.15$, increasing the primary-air fraction concentrated high radiance near the top-mounted burner and shortened the emitting column; secondary-dominant cases produced a longer column. The associated contraction of the oxygen-depleted and CO -rich regions linked this image change to earlier fuel–air mixing and CO conversion.

Excess-air ratio changed both the intensity and spatial extent of the image, although the response was not monotonic across every air split. The $\lambda = 0.60$ series was particularly sensitive to initialisation and included weakly reacting or cold branches; a dark image and low CO in such a case indicate loss of reaction, not efficient burnout. Increasing propane flow at fixed λ generally strengthened and broadened the emitting region, while the highest flow also introduced visible displacement and asymmetry. The flux audit supports this distinction: every air split at $\lambda = 1.00$, 1.15, and 1.623 met the 5% energy-balance criterion, whereas four reacting $\lambda = 0.60$ cases exceeded it and the cold 90/10 branch had essentially no reaction heat release. The 1.5 g s^{-1} fuel case was also marginal at 5.96%; these cases support qualitative branch comparisons rather than absolute thermal conclusions. The nominal $\lambda = 1.00$, 58/41 case also used a different total inlet flow from the other splits and must be rerun before it is used as a controlled air-split comparison.

The 300 K wall case produced the clearest caution for image interpretation. Removing the hot-wall background left a narrow, dark gas-radiation feature even though the oxygen-depleted topology remained. Apparent contraction in an IR image is therefore not necessarily shortening of the chemical flame: gas temperature and composition, wall emission, absorption, and occlusion all contribute to the recorded radiance. Its small mass and energy imbalances (0.0000234% and 0.297%) show that this optical change persists in a well-balanced numerical solution.

Thus, common-scale synthetic IR images can support qualitative discrimination of combustion states within the simulated operating envelope. They cannot by them-

selves identify a unique internal state, and absolute comparison with a physical camera requires measured wall temperatures, numerical-independence checks, and radiometric calibration.

5.1 Recommendations for future work

Future work should reproduce the experimental geometry exactly, repeat the reference and rich cases with documented ignition histories and verified mass and energy balances, and establish CFD and camera-grid independence. The image model should then be calibrated against a physical 1–5 μm camera using measured wall temperatures and identical viewing geometry. Future diagnostic work should retain numerical radiance arrays, calibrated camera metadata, and complete operating families for independent testing.

Bibliography

- [1] S. Colin, F. Normann, C. Fredriksson, and K. Andersson, “Flame Characterization of Cofiring Gaseous and Solid Fuels in Suspensions,” *ACS Omega*, vol. 9, pp. 28268–28282, 2024. doi: 10.1021/acsomega.4c01770.
- [2] E. Ehlme, A. Gunnarsson, E. Fooladgar, F. Normann, and K. Andersson, “An Assessment of Weighted-Sum-of-Grey-Gases Models for Computational Fluid Dynamics Modelling of Hydrogen Flames and Thermal Plasmas in Kilns,” *Applied Thermal Engineering*, vol. 278, Art. no. 127401, 2025. doi: 10.1016/j.applthermaleng.2025.127401.
- [3] S. Colin, F. J. Triana de Las Heras, F. Normann, A. Johansson, J. Fernberg, A. Sepman, J. Wennebro, and H. Wiinikka, “Configuring Hydrogen Lancing to Reduce Carbon and Nitrogen Oxides Emissions from Coal-Fired Rotary Kilns,” *International Journal of Hydrogen Energy*, vol. 120, pp. 323–332, 2025. doi: 10.1016/j.ijhydene.2025.03.322.
- [4] Z. Xi, Z. Fu, X. Hu, S. W. Sabir, and Y. Jiang, “An Investigation on Flame Shape and Size for a High-Pressure Turbulent Non-Premixed Swirl Combustion,” *Energies*, vol. 11, no. 4, Art. no. 930, 2018. doi: 10.3390/en11040930.
- [5] U. Rajak, P. Nashine, P. K. Chaurasiya, and T. N. Verma, “A Numerical Investigation of the Species Transport Approach for Modeling of Gaseous Combustion,” *Journal of Thermal Engineering*, vol. 7, pp. 2054–2067, 2021. doi: 10.14744/jten.2021.0006.
- [6] E. M. Orbegoso, L. F. Figueira da Silva, and R. Serfaty, “Comparative Study of Thermal Radiation Properties Models in Turbulent Non-Premixed Sooting Combustion,” *Numerical Heat Transfer, Part A: Applications*, vol. 69, no. 2, pp. 166–179, 2016. doi: 10.1080/10407782.2015.1052318.
- [7] R. Jarpala, N. V. S. A. Burle, M. Voleti, and R. Sadanandan, “Effect of Swirl on the Flame Dynamics and Pollutant Emissions in an Ultra-Lean Non-Premixed Model Gas Turbine Burner,” *Combustion Science and Technology*, vol. 189, no. 10, pp. 1832–1848, 2017. doi: 10.1080/00102202.2017.1333500.
- [8] A. K. Gupta, D. G. Lilley, and N. Syred, *Swirl Flows*, Abacus Press, Kent, England, 1984.
- [9] J. M. Beer and N. A. Chigier, *Combustion Aerodynamics*, Applied Science Publishers, London, England, 1972.
- [10] K. Wang, J. Fang, J. Wang, S. Zheng, L. Zhao, J. Guan, and Y. Zhang, “A Mixture Fraction-Based Model and Axial Thermal Positions for Buoyancy/Momentum-Controlled Jet Diffusion Flames,” *Combustion Science and Technology*, vol. 192, no. 1, pp. 62–77, 2020. doi: 10.1080/00102202.2018.1556261.

- [11] Z. Abubakar, Y. S. Sanusi, and E. M. A. Mokheimer, “Experimental Analysis of the Stability and Combustion Characteristics of Propane–Oxyfuel and Propane–Air Flames in a Non-Premixed, Swirl-Stabilized Combustor,” *Energy & Fuels*, 2018.
- [12] Z. Abubakar, M. R. Shakeel, and E. M. A. Mokheimer, “Experimental and Numerical Analysis of Non-Premixed Oxycombustion of Hydrogen-Enriched Propane in a Swirl Stabilized Combustor,” 2019.
- [13] N. A. Samiran, K. F. Abu Mansor, R. Abd Rashid, and M. S. Sahul Hamid, “CFD Simulation Analysis of Non-Premixed Combustion Using a Novel Axial-Radial Combined Swirler for Emission Reduction Enhancement,” *CFD Letters*, vol. 15, no. 6, pp. 1–11, 2023.
- [14] B. E. Launder and D. B. Spalding, “The Numerical Computation of Turbulent Flows,” *Computer Methods in Applied Mechanics and Engineering*, vol. 3, no. 2, pp. 269–289, 1974. doi: 10.1016/0045-7825(74)90029-2.
- [15] B. E. Launder, G. J. Reece, and W. Rodi, “Progress in the Development of a Reynolds-Stress Turbulence Closure,” *Journal of Fluid Mechanics*, vol. 68, no. 3, pp. 537–566, 1975.
- [16] M. M. Gibson and B. E. Launder, “Ground Effects on Pressure Fluctuations in the Atmospheric Boundary Layer,” *Journal of Fluid Mechanics*, vol. 86, pp. 491–511, 1978.
- [17] B. E. Launder, “Second-Moment Closure: Present... and Future?,” *International Journal of Heat and Fluid Flow*, vol. 10, no. 4, pp. 282–300, 1989.
- [18] R. Gonçalves dos Santos, S. Ducruix, O. Gicquel, and D. Veynante, “A Study of Three-Dimensional LES of Turbulent Combustion with Radiative Heat Transfer,” *Journal of the Brazilian Society of Mechanical Sciences and Engineering*, vol. 38, pp. 33–48, 2016. doi: 10.1007/s40430-015-0322-8.
- [19] S. Hjærtstam, F. Normann, K. Andersson, and F. Johnsson, “Oxy-Fuel Combustion Modeling: Performance of Global Reaction Mechanisms,” *Industrial & Engineering Chemistry Research*, vol. 51, pp. 10327–10337, 2012. doi: 10.1021/ie300053t.
- [20] K. Andersson, *Characterization of Oxy-Fuel Flames: Their Composition, Temperature and Radiation*, doctoral thesis, Chalmers University of Technology, Gothenburg, Sweden, 2007, ISBN 978-91-7385-006-3.
- [21] A. Kindblom, *From Propane to Hydrogen and Plasma: CFD Modeling of the Transition towards Fossil-Free High-Temperature Systems*, master’s thesis, Chalmers University of Technology, Gothenburg, Sweden, 2026.
- [22] ANSYS, Inc., *ANSYS Fluent User’s Guide*, Release 2024 R2, ANSYS, Inc., Canonsburg, PA, USA, 2024, Chapter 15: Modeling Turbulence.
- [23] ANSYS, Inc., *ANSYS Fluent Theory Guide*, Release 2026 R1, ANSYS, Inc., Canonsburg, PA, USA, 2026, Section 5.3.2: Radiative Transfer Equation.
- [24] D. Bäckström and H. Jilvero, “CFD-Modelling of Chalmers 100 kW Oxy-Fuel Unit: Investigation of Swirling Air and Oxy-Fuel Flames,” Master’s thesis, Chalmers University of Technology, Gothenburg, Sweden, 2009.
- [25] S. A. Orszag, V. Yakhot, S. W. Flannery, F. Boysan, D. Choudhury, J. Maruzewski, and B. Patel, “Renormalization Group Modeling and Turbulence

- Simulations,” in *Proceedings of the International Conference on Near-Wall Turbulent Flows*, Tempe, Arizona, USA, 1993.
- [26] ANSYS, Inc., *ANSYS Fluent Theory Guide*, Release 2024 R2, ANSYS, Inc., Canonsburg, PA, USA, 2024, Chapter 4: Turbulence, including Section 4.3.2: RNG k - ε Model.
 - [27] F. R. Menter, “Two-Equation Eddy-Viscosity Turbulence Models for Engineering Applications,” *AIAA Journal*, vol. 32, no. 8, pp. 1598–1605, 1994.
 - [28] ANSYS, Inc., *ANSYS Fluent Theory Guide*, Release 2025 R1, ANSYS, Inc., Canonsburg, PA, USA, 2025, Section 7.1.1: Volumetric Reactions.
 - [29] W. P. Jones and R. P. Lindstedt, “Global Reaction Schemes for Hydrocarbon Combustion,” *Combustion and Flame*, vol. 73, no. 3, pp. 233–249, 1988. doi: 10.1016/0010-2180(88)90021-1.
 - [30] E. H. Chui and G. D. Raithby, “Computation of Radiant Heat Transfer on a Nonorthogonal Mesh Using the Finite-Volume Method,” *Numerical Heat Transfer, Part B: Fundamentals*, vol. 23, no. 3, pp. 269–288, 1993.
 - [31] T. F. Smith, Z. F. Shen, and J. N. Friedman, “Evaluation of Coefficients for the Weighted Sum of Gray Gases Model,” *Journal of Heat Transfer*, vol. 104, no. 4, pp. 602–608, 1982.
 - [32] T. Ren, M. F. Modest, A. Fateev, G. Sutton, W. Zhao, and F. Rusu, “Machine Learning Applied to Retrieval of Temperature and Concentration Distributions from Infrared Emission Measurements,” *Applied Energy*, vol. 252, Art. no. 113448, 2019. doi: 10.1016/j.apenergy.2019.113448.
 - [33] C. Bong, M. H. A. Ali, S. K. Im, H. Do, and M. S. Bak, “Machine Learning-Based Prediction of Swirl Combustor Operation from Flame Imaging,” *Engineering Applications of Artificial Intelligence*, vol. 138, Art. no. 109374, 2024. doi: 10.1016/j.engappai.2024.109374.
 - [34] M. Dai, B. Zhou, J. Zhang, R. Cheng, Q. Liu, R. Zhao, B. Wang, and B. Gao, “3-D Soot Temperature and Volume Fraction Reconstruction of Afterburner Flame via Deep Learning Algorithms,” *Combustion and Flame*, vol. 252, Art. no. 112743, 2023. doi: 10.1016/j.combustflame.2023.112743.
 - [35] N. B. Erichson, L. Mathelin, Z. Yao, S. L. Brunton, M. W. Mahoney, and J. N. Kutz, “Shallow Neural Networks for Fluid Flow Reconstruction with Limited Sensors,” *Proceedings of the Royal Society A*, vol. 476, Art. no. 20200097, 2020. doi: 10.1098/rspa.2020.0097.
 - [36] A. E. Hoerl and R. W. Kennard, “Ridge Regression: Biased Estimation for Nonorthogonal Problems,” *Technometrics*, vol. 12, no. 1, pp. 55–67, 1970. doi: 10.1080/00401706.1970.10488634.
 - [37] O. Ronneberger, P. Fischer, and T. Brox, “U-Net: Convolutional Networks for Biomedical Image Segmentation,” in *Medical Image Computing and Computer-Assisted Intervention*, pp. 234–241, 2015. doi: 10.1007/978-3-319-24574-4_28.

A

CFD validation against the 2012 oxy-fuel study

A.1 Selection of the validation case

Before the principal simulations of this thesis were performed, a transferred oxy-fuel case was reconstructed from the study by Hjærtstam et al. [19]. This study was selected as the first simulation case because it provides both documented three-dimensional CFD results and experimental measurements of temperature and gas composition. It therefore offered a useful benchmark for checking the reconstructed furnace geometry, inlet definitions, species transport, global chemistry implementation, thermal boundary conditions, and the extraction of axial and radial profiles.

Hjærtstam et al. investigated the Chalmers 100 kW oxy-fuel unit using a propane-fired OF27 flame. Three global mechanisms developed for oxy-fuel conditions—the three-step, four-step, and six-step mechanisms—were compared with experimental data and two additional references. These were the Jones–Lindstedt (JL) mechanism and a detailed one-dimensional plug-flow mechanism. The paper showed that the selected global reaction mechanism has a strong effect on the calculated flame temperature and the formation and burnout of CO. In the original CFD results, the JL mechanism produced a short and intense flame with the highest centreline temperature, whereas the oxy-fuel mechanisms generally produced smoother axial temperature gradients and longer CO-rich regions. The authors concluded that the JL mechanism gave the most physically consistent CO reaction history and was the preferable global alternative when a detailed mechanism was computationally impractical.

The terminology of the source paper is retained here: the JL mechanism and the six-step oxy-fuel mechanism are separate reaction schemes. The transferred Fluent calculation assessed in this appendix uses the six-step scheme under the OF27 operating conditions. The JL curve digitized from the paper is retained in the supporting data, but it is intentionally omitted from the appendix figures so that the comparison shows only the present Fluent result and the measured data.

A.2 Transferred operating and boundary conditions

The experimental case had an 80 kW propane heat input and used dry flue-gas recycling. The CFD boundary conditions in the 2012 study idealised the oxidiser as 27 vol.% O₂ and 73 vol.% CO₂ and the fuel as pure propane. The principal quantities transferred to the validation setup are summarised in Table A.1.

Table A.1: Principal OF27 operating and boundary conditions adopted from Hjærtstam et al. [19].

Quantity	Value or modelling assumption
Fuel and thermal input	Propane; 1.74 g s ⁻¹ ; 80 kW
Oxidiser composition used in CFD	27 vol.% O ₂ and 73 vol.% CO ₂
Feed-gas temperature	25–30 °C
Primary and secondary feed-gas flows	29.5 and 42 m _n ³ h ⁻¹ , respectively
Stoichiometric ratio	1.15
Primary and secondary register angles	45° and 15°, respectively
Cooling-water flow and measured heat absorption	3.75 m ³ h ⁻¹ and 52 kW
Cooling-tube surface temperature in CFD	Fixed at 10 °C
Furnace-wall treatment in the source CFD model	Adiabatic, opaque walls with emissivity equal to one
Fuel-injection direction	Approximately 45° to the furnace centreline

The original paper modelled one quarter of the furnace with periodic boundary conditions and one of the four symmetrically placed cooling tubes. Its mesh contained approximately 340,000 hexahedral cells. The Realizable k – ε model was combined with the Eddy Dissipation Concept for turbulence–chemistry interaction. Radiation was treated using the Discrete Ordinates Method and an oxy-fuel weighted-sum-of-grey-gases model. A steady segregated solver, SIMPLE pressure–velocity coupling, second-order upwind discretisation, and in-situ adaptive tabulation were used. These details define the numerical context of the published reference results; the present work uses the reconstructed computational domain and mesh described in Chapter 3, while retaining the paper’s OF27 operating conditions as the validation basis.

A.3 Comparison with the experimental profiles

The experimental values used below were digitised from the measurement markers in Figures 8 and 9 of Hjærtstam et al. [19]. Temperature is reported in degrees

Celsius, while the CO concentration is expressed as dry volume percent. The axial profiles follow the furnace centreline, and the radial profiles correspond to a plane 0.384 m downstream of the burner inlet. Because the measurements were recovered from raster plots, the numerical values and the error measures derived from them should be regarded as approximate.

Temperature validation: Fluent and experiment

Experimental markers digitized from the supplied plots; published model curves are excluded.

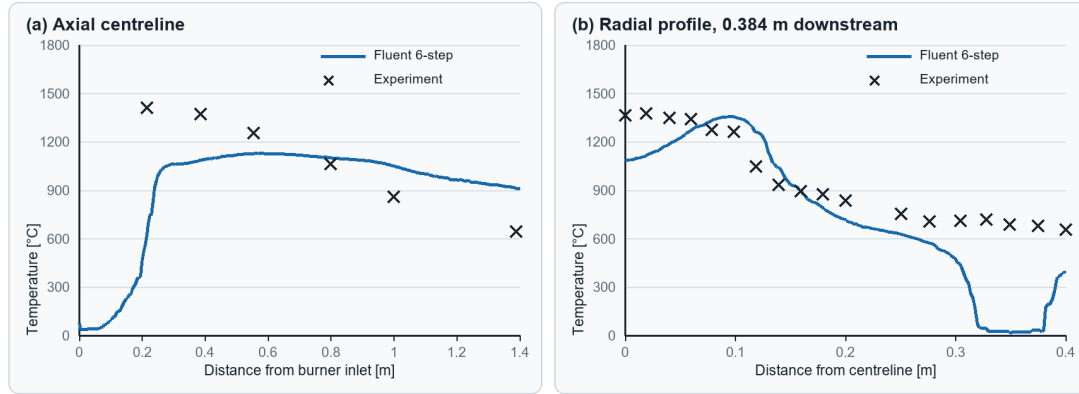


Figure A.1: Comparison of the Fluent temperature predictions with the digitized experimental measurements along the furnace centreline and on a radial profile 0.384 m downstream of the burner inlet.

The present six-step calculation predicts a later centreline temperature rise and a lower temperature through much of the main combustion region than the measurements. The agreement improves farther downstream as the calculated and measured temperatures approach the post-flame level. In the radial profile, the calculated temperature initially rises towards a maximum near 0.1 m from the centreline and then decreases more rapidly than the measurements. The pronounced reduction near the outer radius is associated with the cooled structures and the wall region sampled by the reconstructed three-dimensional line. Based on the digitised measurement locations, the temperature root-mean-square errors are approximately 366 °C for the axial profile and 313 °C for the radial profile.

CO validation: Fluent and experiment

Experimental markers digitized from the supplied plots; published model curves are excluded.

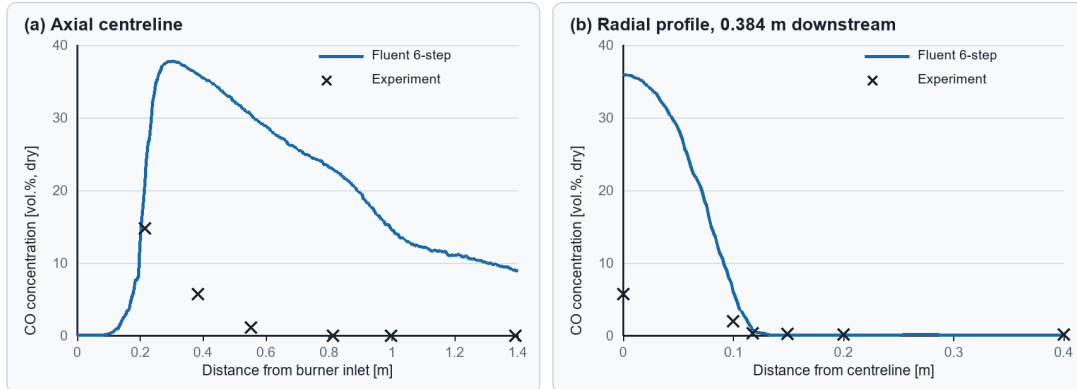


Figure A.2: Comparison of the Fluent dry CO concentration predictions with the digitized experimental measurements along the furnace centreline and on a radial profile 0.384 m downstream of the burner inlet.

The largest discrepancy is observed for CO. The Fluent calculation predicts a strong CO peak and a substantially longer CO-rich zone than the measurements. Along the centreline, the calculated dry CO concentration remains appreciable at the downstream end of the comparison range, whereas the measured values are close to zero after approximately 0.8 m. The radial calculation also overpredicts CO near the centreline, although both calculation and experiment show a rapid reduction with increasing radial distance. The corresponding approximate root-mean-square errors are 20.9 percentage points for the axial profile and 12.5 percentage points for the radial profile.

These results show that the transferred case was useful as an implementation and workflow check but did not provide quantitative validation of the retained six-step setup. The disagreement is consistent with the sensitivity identified in the 2012 paper: temperature and CO depend not only on the global kinetic scheme but also on turbulence–chemistry interaction, radiation, cooling, inlet mixing and swirl, mesh resolution, and convergence. The comparison was therefore used to identify modelling aspects requiring further assessment before the principal simulations were evaluated.

B

CFD comparison with the 2024 pure-propane measurements

B.1 Selection and scope of the comparison

The principal experimental reference for the propane simulations is the study by Colin et al. [1]. The authors mapped the in-flame gas composition in the Chalmers 100 kW unit for three fuel conditions: 100% lignite, a 50/50 propane–lignite mixture, and 100% propane. The mapping cases were operated at an 80 kW thermal input and a stoichiometric ratio of 1.15. Gas samples were collected through ports M2–M5. Carbon monoxide was measured as part of the wet-gas FTIR analysis, whereas oxygen was measured with a natural-gas analyser. For the 100% propane mapping case, combustion air was introduced through the two outer air registers and no transport air was used.

The present Fluent solution also uses 100% propane and contains no lignite. The case identifier 41/58 denotes the nominal percentage split of the total 31.01 g s^{-1} combustion-air mass flow between the burner air streams; it is not a propane/lignite ratio. The global fuel basis, stoichiometric ratio, and total air mass flow are therefore aligned with the paper’s 100% propane reference. The experimental mapping case was operated without transport air. Quantitative agreement must still be interpreted with respect to the detailed air-register implementation, inlet momentum, wall treatment, wet/dry concentration basis, and sampling procedure.

B.2 Extraction and reconstruction of the concentration fields

The experimental CO and O₂ contour maps were taken from Figure 5(c) of Colin et al. [1]. The corresponding radial average, minimum, and maximum values were recovered from the vector objects in Figure 6(c)(2–3). The four plotted series P2–P5 were retained in their drawing order and identified with measurement ports M2–M5. The reported horizontal positions were 0, 10, 20, 25, 30, 35, 40, 45, 50, 55, 60, 70, and 80 cm. This vector-based extraction avoids the larger coordinate uncertainty associated with digitising a raster image, although the reconstructed values should still be regarded as approximate representations of the published plots.

The Fluent species fields were read directly from the paired `cas.h5/dat.h5` solution files. Cell-based species mass fractions were reconstructed to points on the $x =$

0 mid-plane and converted to mole fractions using the molecular weights of the seven transported species. The contour coordinate system was transformed to the experimental 80×80 cm view according to $x_{\text{plot}} = (y + 0.4) 100$ and $z_{\text{plot}} = (z - 0.4) 100$. Radial profiles were then extracted at $z = 0.615, 0.815, 0.984$, and 1.201 m, corresponding to M2–M5.

B.3 Comparison of CO and oxygen contours

Figure B.1 compares the published 100% propane contours with the newly extracted 100% propane Fluent fields. The CFD case uses a nominal 41%/58% split of the total 31.01 g s^{-1} air mass flow. Common display limits of 0–6 vol.% for CO and 0–10 vol.% for O_2 are used so that the spatial distributions can be compared directly. Values above the upper limit are saturated in the Fluent panels.

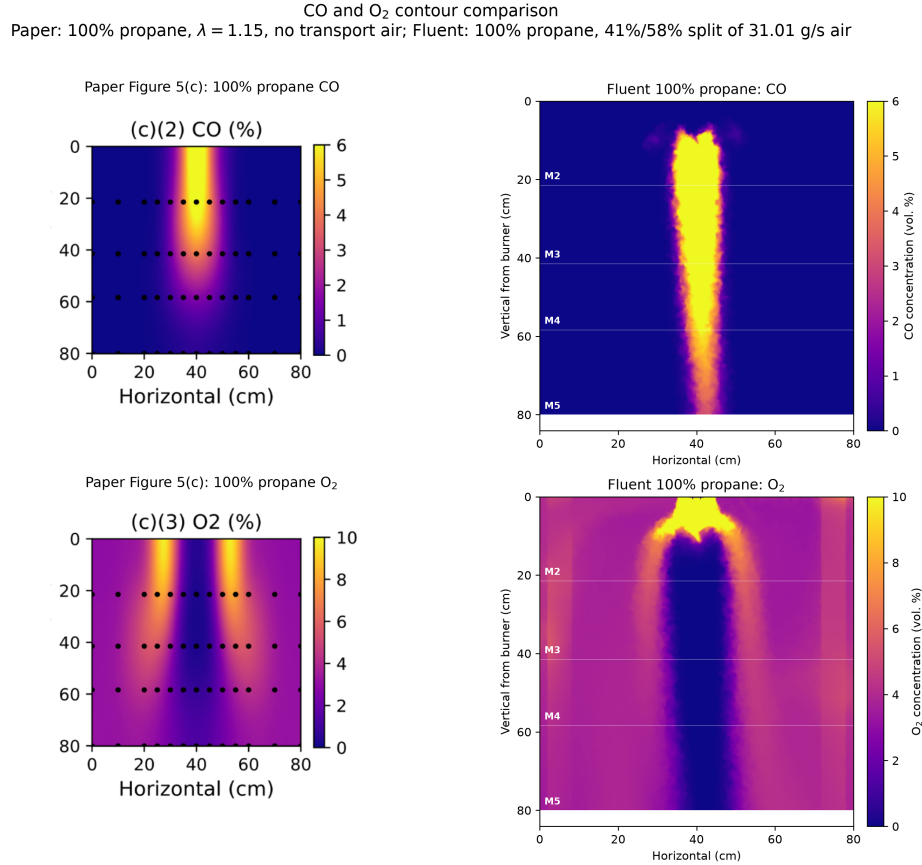


Figure B.1: Comparison of the experimental 100% propane CO and O_2 contours reported by Colin et al. [1] with the present 100% propane Fluent solution. The CFD case identifier 41/58 refers to the combustion-air split and not to the fuel composition.

Both cases show a CO-rich region near the furnace centreline and a corresponding oxygen-depleted core. In the experimental propane flame, the CO region is nar-

row and its concentration decreases strongly between M2 and M5. The Fluent field retains a longer, more concentrated centreline plume. At M2, the calculated maximum CO concentration is approximately 11.42 vol.%, decreasing to approximately 3.30 vol.% at M5. The paper's centreline average decreases from approximately 3.68 vol.% at M2 to 0.17 vol.% at M5.

The oxygen fields show a related difference. The pure-propane experiment has two oxygen-rich lobes on either side of the depleted core near M2. At horizontal positions of approximately 30 and 50 cm, the published M2 average is about 13.75 vol.% and the maximum is close to 15 vol.%. In the Fluent solution, the largest O₂ value on the M2 profile is about 5.79 vol.%. The calculated oxygen-depleted core persists farther downstream, consistent with the slower CO burnout seen in the Fluent field.

B.4 Axial profiles at 30, 35, and 40 cm

The contour comparison is complemented by axial profiles along the three vertical sampling lines located 30, 35, and 40 cm from the side of the furnace. The horizontal coordinate in Figures B.2 and B.3 is the distance from the burner exit. The black markers are the 2024 pure-propane measurements at M2–M5, whereas the continuous curves are extracted from the Fluent solution. The oxygen plots include both retained turbulence-model predictions; the available CO comparison contains the RNG $k-\varepsilon$ result.

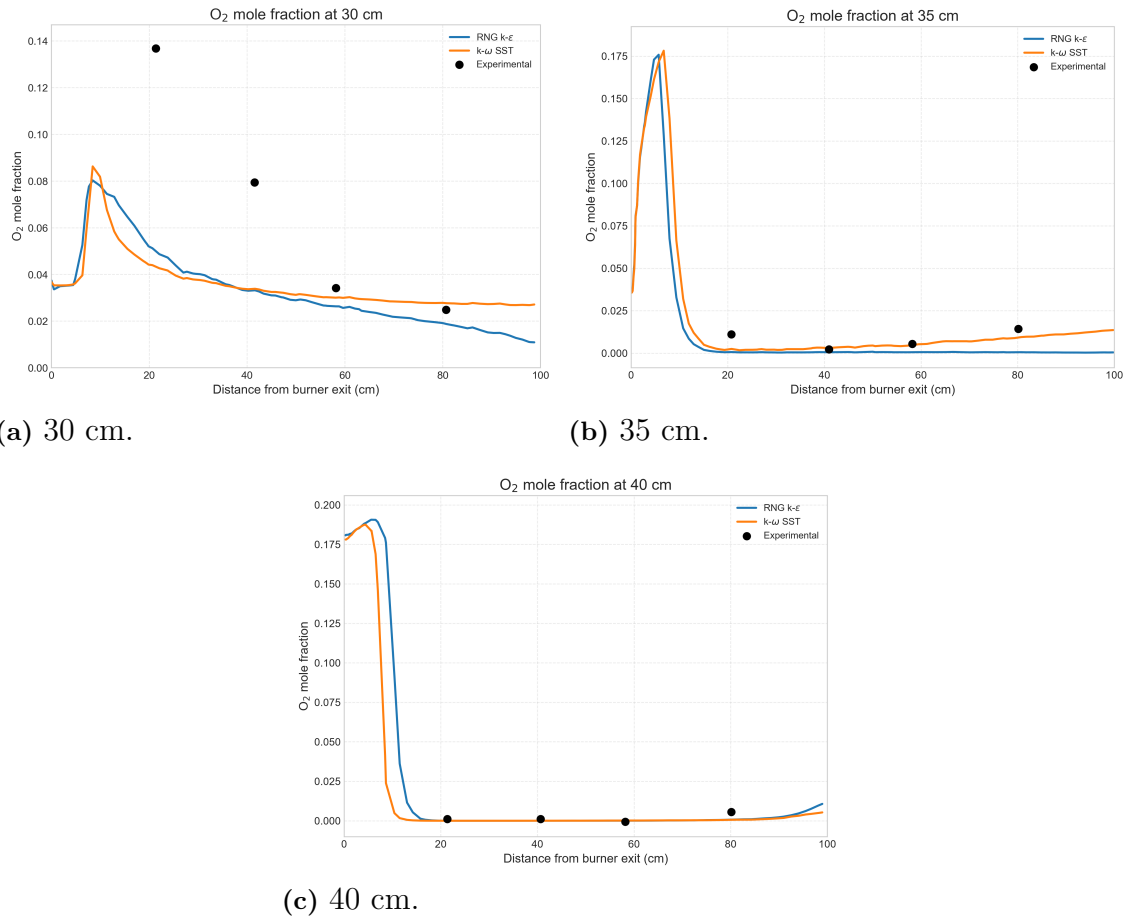


Figure B.2: Axial O_2 mole-fraction profiles on the 30, 35, and 40 cm sampling lines for the 100% propane Fluent case, compared with the 2024 pure-propane measurements of Colin et al. [1].

At 30 cm, both CFD curves reproduce the oxygen rise and axial decay but underpredict the first two measurements. On the 35 and 40 cm lines, the high near-burner oxygen region collapses before M2; the low downstream measurements are therefore qualitatively consistent with an oxygen-depleted reaction zone. Most clearly at 35 cm, the divergence between the RNG $k-\varepsilon$ and $k-\omega$ SST curves shows that the predicted oxygen recovery is sensitive to the turbulence closure.

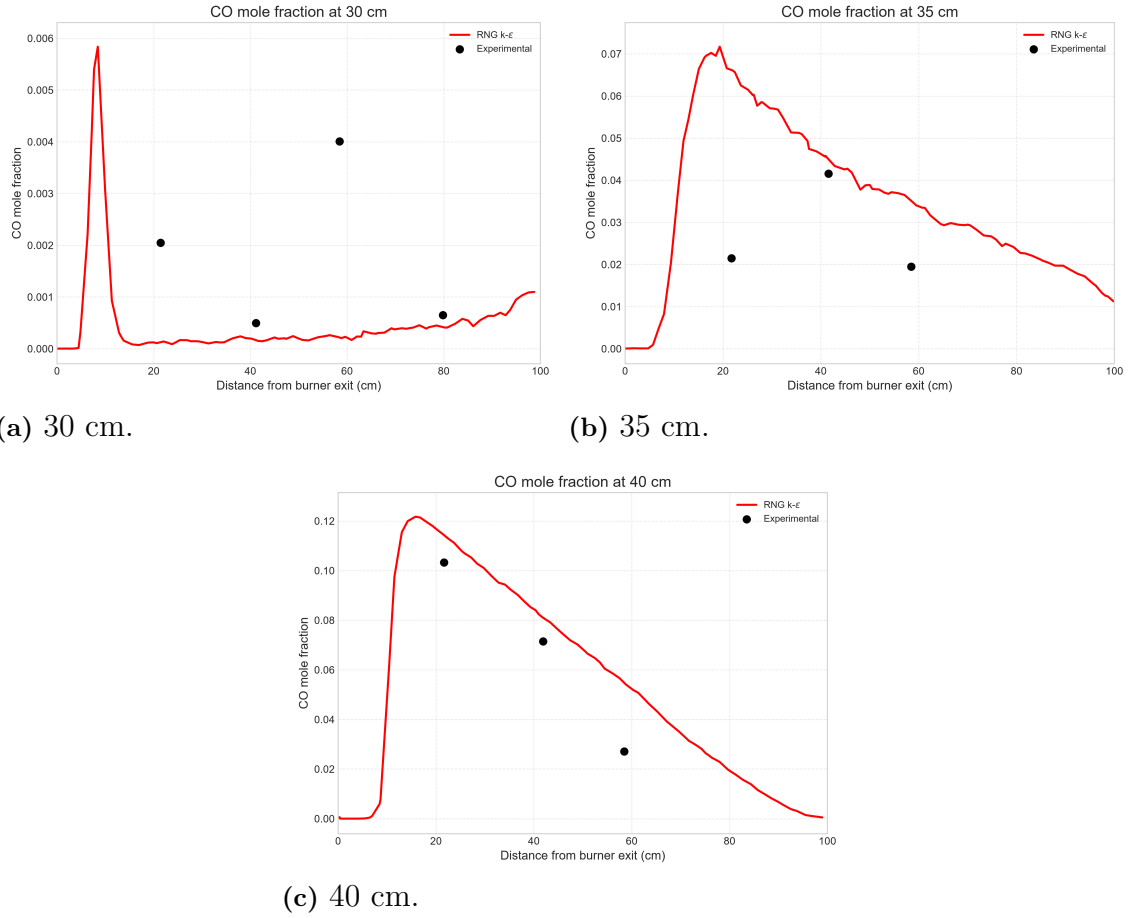


Figure B.3: Axial CO mole-fraction profiles on the 30, 35, and 40 cm sampling lines for the 100% propane Fluent case, compared with the 2024 pure-propane measurements of Colin et al. [1].

The CO profiles provide the complementary view of the oxygen-depleted core. At 30 cm, the CFD field produces a narrow near-burner CO peak, while the measured points indicate that the local CO distribution is not reproduced uniformly along the full line. At 35 and 40 cm, the calculation predicts broader CO-rich regions followed by a gradual downstream decrease. The 40 cm curve captures the measured downstream reduction more closely near the first sampling ports, whereas the 35 cm curve overpredicts the near-burner CO level and retains CO over a longer axial distance. Considered together with the oxygen profiles, these results indicate that the CFD model captures the inverse relationship between oxygen depletion and CO formation but predicts a reaction core whose position and persistence differ from the 2024 measurements.

B.5 Radial profiles at M2–M5

Figures B.4 and B.5 compare the complete Fluent radial profiles with the paper averages and minimum-to-maximum ranges. The solid curves denote the Fluent solution, while the open markers and vertical bars denote the published average and range, respectively.

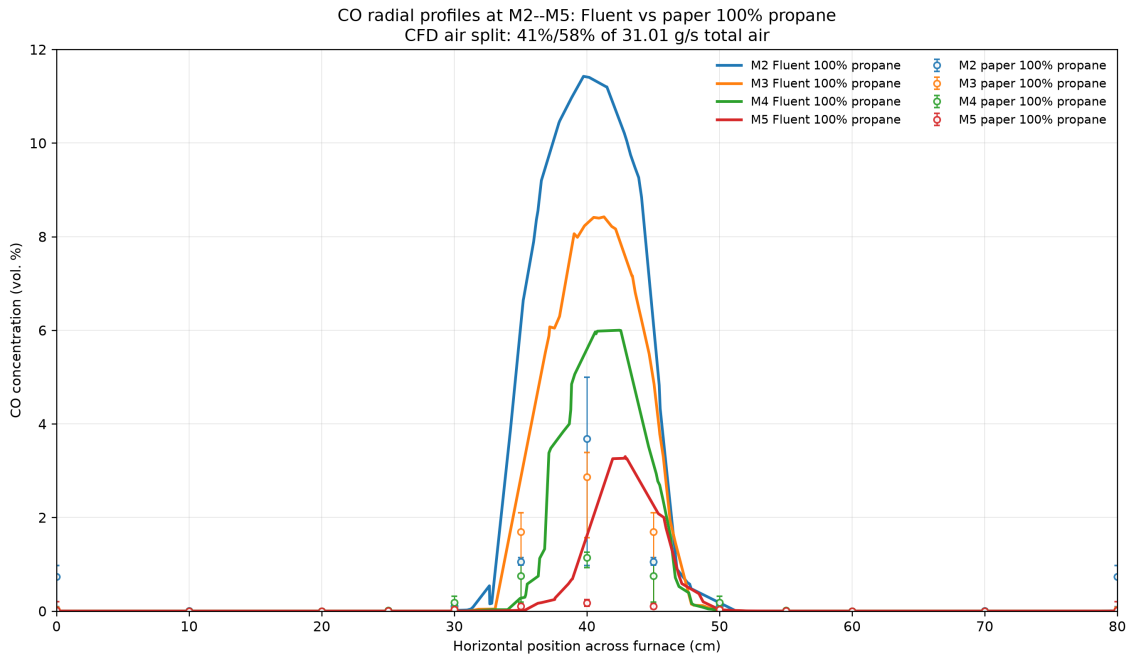


Figure B.4: Radial CO profiles at M2–M5 for the 100% propane Fluent case, using the nominal 41%/58% air split, compared with the average and minimum-to-maximum range reconstructed from the 100% propane measurements of Colin et al. [1].

The calculated CO peaks decrease monotonically downstream, from approximately 11.42 vol.% at M2 to 8.42, 6.00, and 3.30 vol.% at M3, M4, and M5, respectively. The corresponding length-weighted radial averages are 1.41, 0.95, 0.57, and 0.25 vol.%. The experiment shows the same downstream reduction, but with lower and narrower CO peaks. Since both cases use 100% propane, the difference indicates an overextended reaction zone in the present calculation or a remaining mismatch in the air injection, thermal boundary conditions, concentration basis, or sampling procedure.

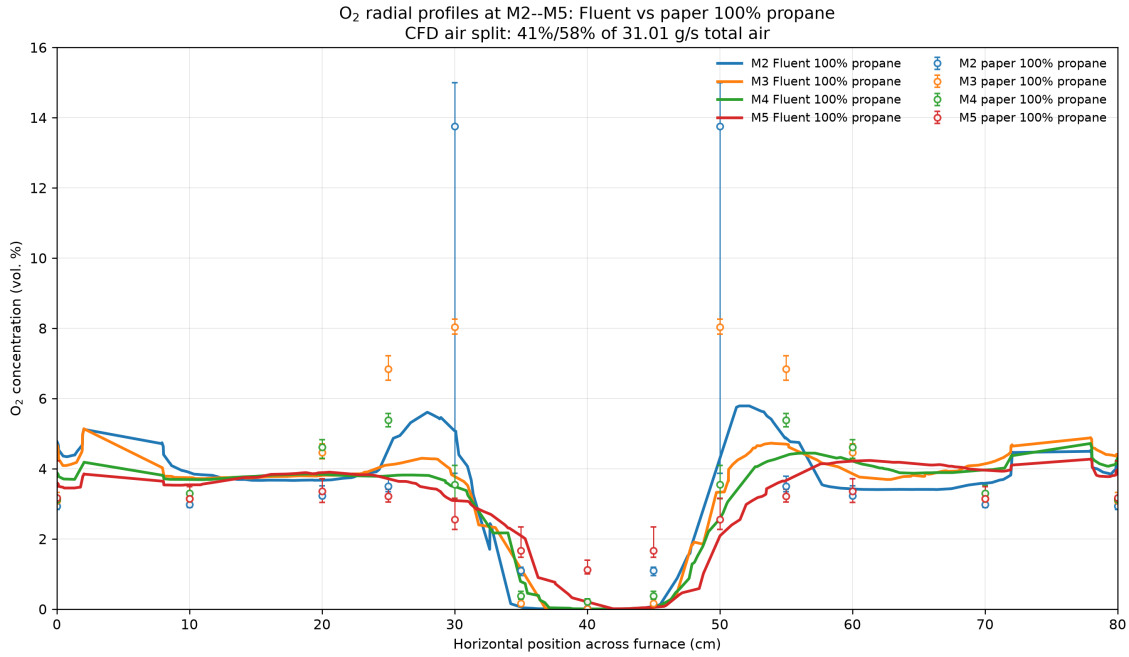


Figure B.5: Radial O_2 profiles at M2–M5 for the 100% propane Fluent case, using the nominal 41%/58% air split, compared with the average and minimum-to-maximum range reconstructed from the 100% propane measurements of Colin et al. [1].

The Fluent O_2 profiles reproduce the qualitative centreline depletion observed in the measurements. Their length-weighted radial averages vary only slightly, from 3.41 vol.% at M2 to 3.11 vol.% at M5. In contrast, the experimental M2 profile exhibits much stronger oxygen-rich side lobes and a more abrupt radial transition into the depleted centre. Downstream, the measured profiles become flatter and the difference between the experiment and the Fluent field decreases outside the central reaction zone.

Overall, the comparison supports the qualitative flame topology predicted by the model: CO is concentrated around an oxygen-depleted core and decreases with distance from the burner. Quantitatively, the Fluent solution overpredicts the persistence and peak level of CO and underpredicts the strong M2 oxygen lobes of the published propane flame. These deviations are not caused by a propane/lignite mismatch, because both the CFD and experimental cases use 100% propane. They should instead be assessed against the turbulence–chemistry closure, radiation and wall treatment, mesh resolution, air-register split, transport-air treatment, wet/dry concentration basis, and sampling locations. Formal validation metrics become meaningful once these remaining boundary and measurement definitions have been confirmed to be equivalent.

B.5.1 Mesh-resolution assessment

Several grids were generated during model development. Their nominal cell counts and recorded local controls are shown in Table B.1. The labels coarse, medium, and

fine refer to the development cases and should not be interpreted solely from the global maximum size, because the local vane, injector, outlet, and prism settings controlled much of the final cell count.

Table B.1: Mesh variants retained from the grid-development study. Cell counts for the development grids are nominal values indicated by the archived case names.

Grid	Cells	Global max.	Vanes	Injector	First prism
Coarse	~ 0.7 mil- lion	200 mm	12 mm	12 mm	0.10 mm
Medium	~ 2.9 mil- lion	12.5 mm	1 mm	1 mm	0.10 mm
Fine	~ 5.4 mil- lion	15 mm	0.5 mm	0.5 mm	0.10 mm
Final	2.096 mil- lion	15 mm	1 mm	1 mm	0.05 mm

The mesh assessment used quantities connected to the study objectives rather than residuals alone. These included the axial temperature development, peak and volume-averaged temperature, oxygen and carbon-monoxide levels at the comparison locations, flame length and shape, pressure loss, and the strength and extent of the central recirculation zone. Contour plots were also checked for grid imprinting and discontinuities at size transitions. The final mesh was adopted as a compromise between local resolution of the burner passages and the cost of the complete turbulence and parametric case matrix.

C

Numerical-resolution and camera-model checks

This appendix retains the numerical checks that support the modelling choices without interrupting the image-centred Results chapter. The checks quantify discretisation sensitivity; they are not additional operating-condition results.

C.1 Reacting-flow mesh resolution

Reacting solutions at $\lambda = 1.15$ were compared on grids containing 769,058, 2,096,226, and 2,930,451 cells. The observables were selected to test the quantities used later in the thesis: axial temperature development and radial O_2 and CO profiles at M2–M5. Figure C.1 shows that all grids retain the same broad flame topology, but their curves do not collapse to a common solution.

The mean absolute difference in axial temperature decreased from 217.9 K between the two coarser solutions to 85.6 K between the two finer solutions. The largest local difference between the finer grids remained 1282.9 K near the steep flame-front region, however. The peak centreline temperature changed from 1941 K on the intermediate grid to 1824 K on the finest grid, while the mean of the M2–M5 CO maxima increased from 47,393 to 74,784 ppmv. Agreement in peak temperature therefore did not imply convergence of the reacting species field. The retained-grid results are consequently interpreted as mesh-resolved parametric trends rather than formally grid-converged values.

Figures C.2–C.5 provide the individual plots underlying the compact comparison in Figure C.1. They are retained here so that the displacement of the flame front and the local species sensitivity can be inspected without reducing four radial stations to a single scalar measure.

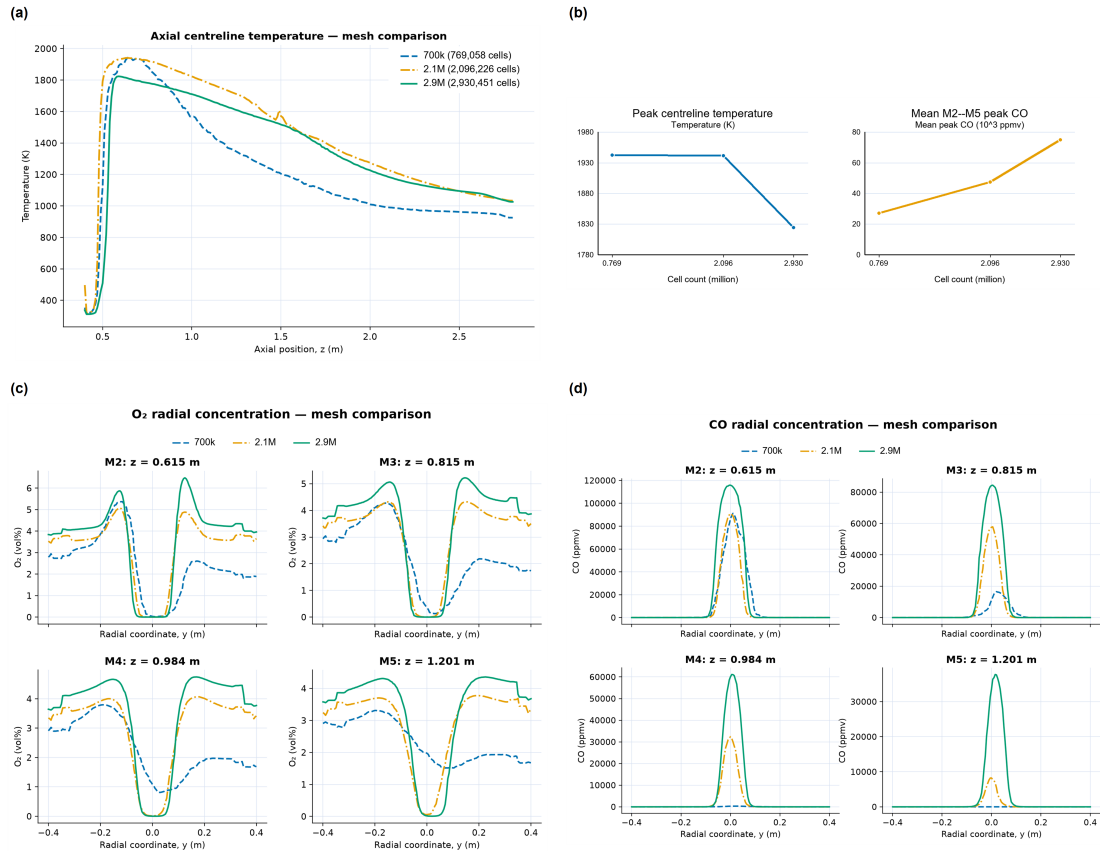


Figure C.1: Mesh-resolution assessment using axial temperature and radial O₂/CO observables at $\lambda = 1.15$.

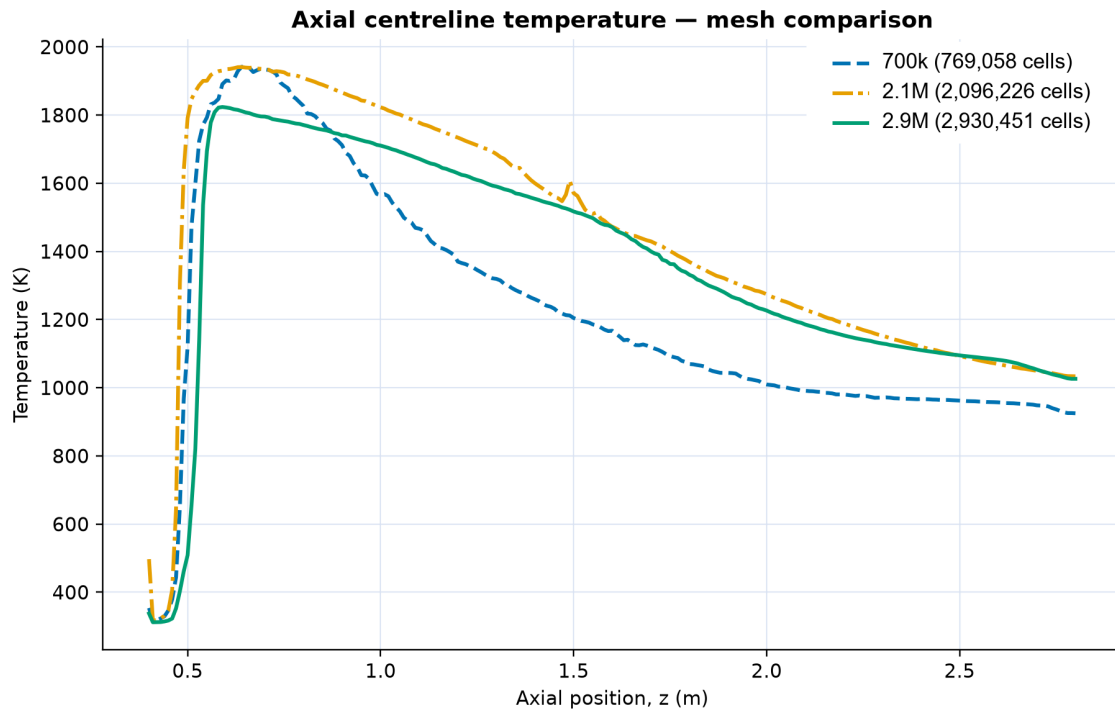


Figure C.2: Detailed axial centreline-temperature comparison for the three reacting-flow meshes. The finest grid shifts the rapid temperature rise downstream and predicts a lower peak, while the two finer solutions become similar only in the later part of the furnace.

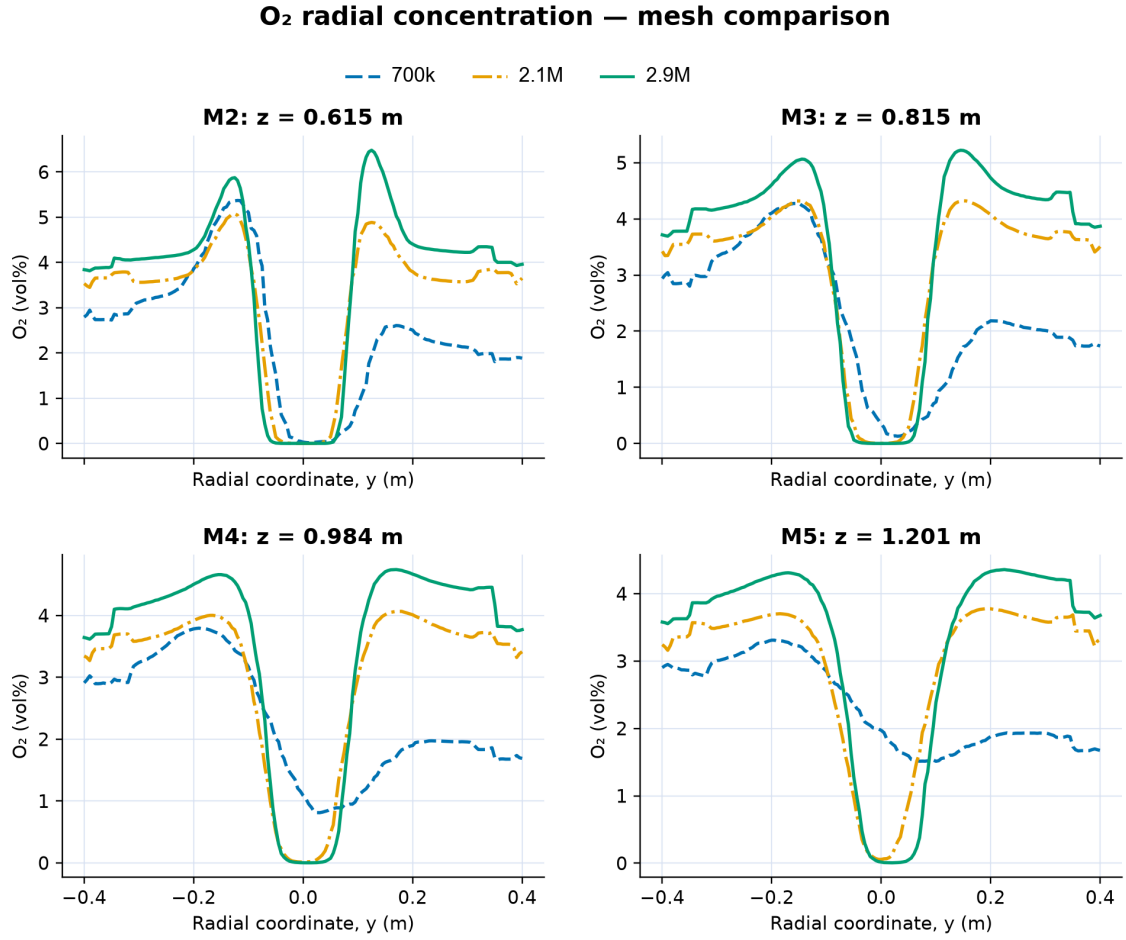


Figure C.3: Detailed radial O₂ profiles at M2–M5 for the mesh-resolution assessment. All grids retain an oxygen-depleted centre, but the predicted shoulder magnitude, core width, and downstream recovery remain mesh-sensitive.

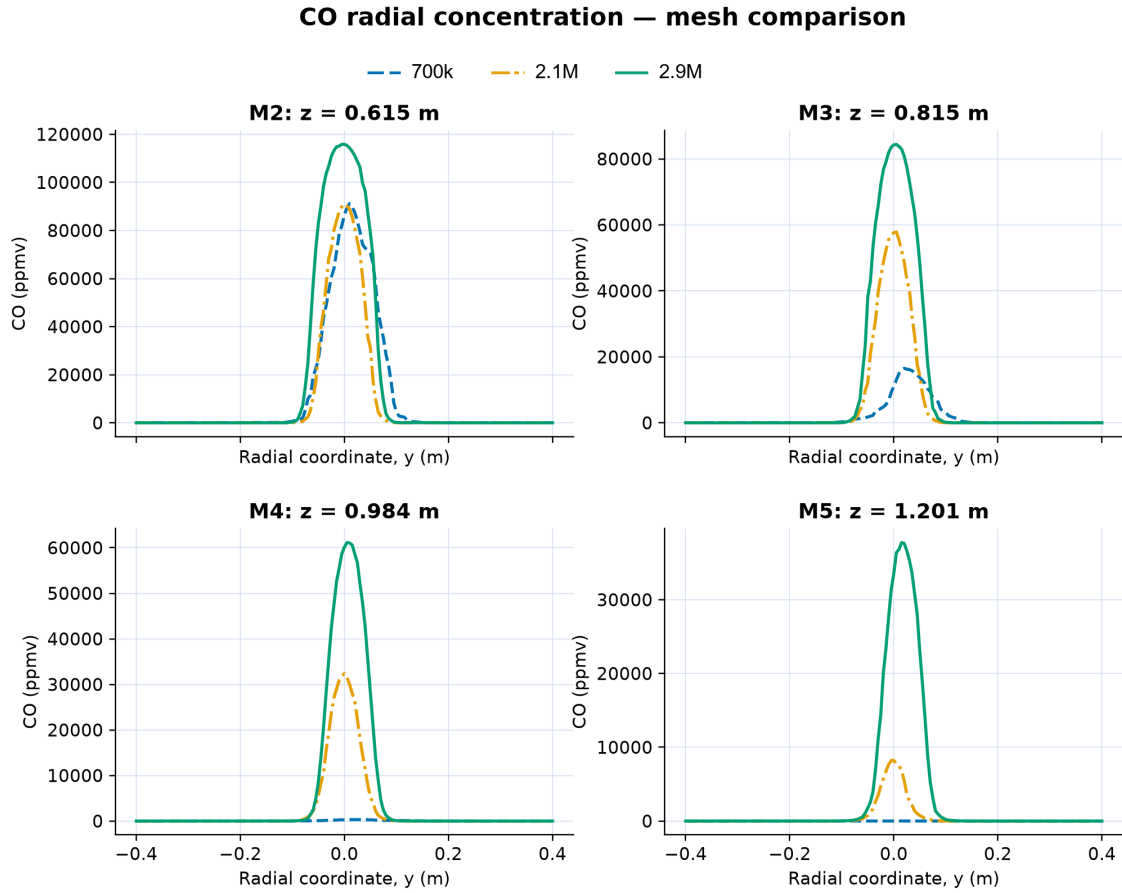


Figure C.4: Detailed radial CO profiles at M2–M5 for the mesh-resolution assessment. Refinement substantially increases the centreline CO peaks, particularly downstream, demonstrating that temperature agreement alone is not sufficient evidence of species-field convergence.

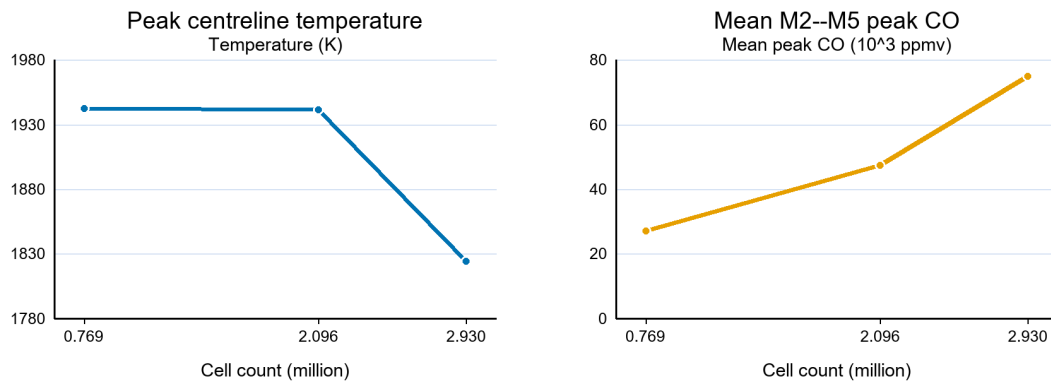


Figure C.5: Scalar summary of mesh sensitivity. Peak centreline temperature decreases on the finest grid whereas the mean M2–M5 peak CO concentration increases monotonically with cell count.

C.2 Virtual-camera numerical checks

The optimised and original camera implementations were evaluated using identical CFD rays and spectral data. Ray paths were identical, interpolated SNBM parameters showed no difference, and the largest relative differences in emissive-cell and final-intensity values were approximately 2.6×10^{-15} and 4×10^{-16} , respectively. For a 50×50 -pixel, 449-band input table, optimisation reduced the recorded execution time from approximately 26.5 minutes to 16 seconds on two processor cores without changing the numerical result.

Reducing the ray-marching increment from 0.01 to 0.002 m changed mean intensity by approximately 0.2%. Refining the cylindrical interpolation grid from $10 \times 32 \times 50$ to $20 \times 64 \times 100$ changed mean intensity by approximately 8%. The ray increment was therefore adequate for the tested view, whereas interpolation-grid resolution remained the dominant numerical uncertainty in the camera post-processing. Quantitative image comparisons use the refined grid where available; coarser images are interpreted by spatial structure rather than absolute radiance.

D

Supplementary parametric-study images

D.1 Steady-state and flux-balance audit

Table D.1 applies the acceptance measures defined in the methodology to every non-master parametric case/data pair. The master case is reported separately in Section 3.3.1. The reaction heat is the volume-integrated chemical-energy source, $\dot{Q}_{\text{out}}$ is the net flow-boundary enthalpy plus heat removed at walls, and $\dot{Q}_{\text{net}} = \dot{Q}_{\text{out}} - \dot{Q}_{\text{reaction}}$. The sign of $\dot{Q}_{\text{net}}$ indicates which side of the balance is larger; acceptance is based on its magnitude relative to the larger energy rate. “Qual.” marks cases above the adopted 5% energy-error limit.

Table D.1: Mass and energy convergence audit for the parametric calculations.

Family	Case	Iter.	ε_m (%)	$\dot{Q}_{\text{reaction}}$ (kW)	$\dot{Q}_{\text{out}}$ (kW)	$\dot{Q}_{\text{net}} / \varepsilon_E$ (kW / %)	Status
Excess air	$\lambda = 0.60, 10/90$	11925	0.0032	48.88	53.47	4.59 / 8.59	Qual.
	$\lambda = 0.60, 25/75$	12252	2.11×10^{-7}	48.31	51.13	2.82 / 5.52	Qual.
	$\lambda = 0.60, 41/58$	12097	0.0059	49.02	51.89	2.87 / 5.53	Qual.
	$\lambda = 0.60, 58/41$	44246	0.0025	40.62	40.78	0.17 / 0.40	Pass
	$\lambda = 0.60, 75/25$	12165	0.0085	19.61	53.59	33.97 / 63.40	Qual.
	$\lambda = 0.60, 90/10$	29535	0.0003	3.92×10^{-6}	0.65	0.65 / 100.00	Qual.
	$\lambda = 1.00, 10/90$	22689	4.75×10^{-5}	82.26	83.11	0.85 / 1.02	Pass
	$\lambda = 1.00, 25/75$	20212	0.0010	82.17	82.87	0.70 / 0.85	Pass
	$\lambda = 1.00, 41/58$	17681	0.0002	82.47	83.49	1.03 / 1.23	Pass
	$\lambda = 1.00, 58/41$	26685	0.0008	84.25	86.31	2.06 / 2.39	Pass
	$\lambda = 1.00, 75/25$	23841	2.57×10^{-6}	83.27	82.15	-1.12 / 1.34	Pass
	$\lambda = 1.00, 90/10$	28500	0.0003	82.12	81.75	-0.38 / 0.46	Pass
	$\lambda = 1.15, 10/90$	21032	0.0004	83.76	84.44	0.68 / 0.81	Pass
	$\lambda = 1.15, 25/75$	20561	0.0002	84.63	83.86	-0.77 / 0.91	Pass
	$\lambda = 1.15, 58/41$	27132	0.0002	85.46	84.40	-1.06 / 1.24	Pass
	$\lambda = 1.15, 75/25$	21579	4.46×10^{-5}	88.00	88.00	-0.00 / 0.00	Pass
	$\lambda = 1.15, 90/10$	30708	6.34×10^{-5}	86.09	86.96	0.87 / 1.01	Pass
	$\lambda = 1.623, 10/90$	24746	8.02×10^{-5}	89.66	89.87	0.22 / 0.24	Pass
	$\lambda = 1.623, 25/75$	28417	0.0002	89.19	89.96	0.76 / 0.85	Pass
	$\lambda = 1.623, 41/58$	28771	2.72×10^{-5}	98.81	95.98	-2.83 / 2.86	Pass
Fuel flow	$\lambda = 1.623, 58/41$	24571	8.14×10^{-5}	93.46	92.43	-1.03 / 1.10	Pass
	$\lambda = 1.623, 75/25$	31025	0.0001	90.45	90.90	0.45 / 0.49	Pass
	$\lambda = 1.623, 90/10$	27033	0.0002	90.32	91.68	1.37 / 1.49	Pass
	1.0 g s ⁻¹	15654	0.0010	47.78	49.56	1.78 / 3.60	Pass
	1.5 g s ⁻¹	22987	9.73×10^{-5}	77.75	73.12	-4.63 / 5.96	Qual.
Wall temp.	2.0 g s ⁻¹	24903	8.58×10^{-6}	96.86	97.12	0.26 / 0.27	Pass
	3.0 g s ⁻¹	16140	0.0001	146.76	151.56	4.80 / 3.17	Pass
	300 K	42319	2.34×10^{-5}	81.09	80.85	-0.24 / 0.30	Pass

All cases close mass tightly: ε_m ranges from $2.11 \times 10^{-7}\%$ to 0.00850%. Final continuity residuals range from 1.40×10^{-4} to 2.25×10^{-3} , and final energy residuals

from 5.46×10^{-6} to 1.00×10^{-4} . These residual and mass results alone do not establish a reacting steady state. Twenty-two of the 28 non-master cases also satisfy the 5% energy criterion. The exceptions concentrate in the rich $\lambda = 0.60$ series and in the 1.5 g s^{-1} fuel case.

The $\lambda = 0.60$, 75/25 case is the strongest reacting outlier: its reaction source falls to 19.61 kW while the calculated output remains 53.59 kW, producing a 63.40% error. The 90/10 case is more decisive physically: its reaction source is only 3.92×10^{-6} kW, consistent with the approximately 307 K cold branch rather than a converged flame. The 10/90, 25/75, and 41.15/58.85 rich cases are closer but still exceed the quantitative threshold. The 1.5 g s^{-1} fuel case is marginal at 5.96%. Conversely, the 300 K wall case closes energy to 0.297%, showing that its dark infrared appearance is a physical consequence of the imposed thermal boundary rather than poor global balance. One setup inconsistency is also visible independently of convergence: the $\lambda = 1.00$, 58/41 file has a total inlet flow of $0.033508 \text{ kg s}^{-1}$, whereas the other five files at that nominal excess-air ratio have $0.028730 \text{ kg s}^{-1}$. Its mass balance closes to 0.000785%, but it does not represent the same total-flow condition and should not be used as a strict air-split comparison until its inlet settings are corrected and rerun.

This appendix retains supporting images that are not displayed in the Results chapter. The six air-split cases at $\lambda = 1.15$, the complete propane-flow comparison, and the adiabatic/300 K wall-temperature comparison are already shown in Results as complete multi-panel figures and are therefore not repeated here. Likewise, the $\lambda = 0.60$ infrared images are omitted because all six appear in Figures 4.22 and 4.23. The plates below contain the remaining temperature fields and infrared views needed to document the excess-air-ratio matrix without duplicating the principal comparisons.

D.2 Temperature fields across excess-air ratio

Figures D.1– D.3 provide the temperature contours for all six primary/secondary air splits at $\lambda = 0.60$, 1.00, and 1.623. Each panel retains the scale exported for that calculation; comparisons of topology and flame extent are therefore more reliable than comparisons based only on colour.

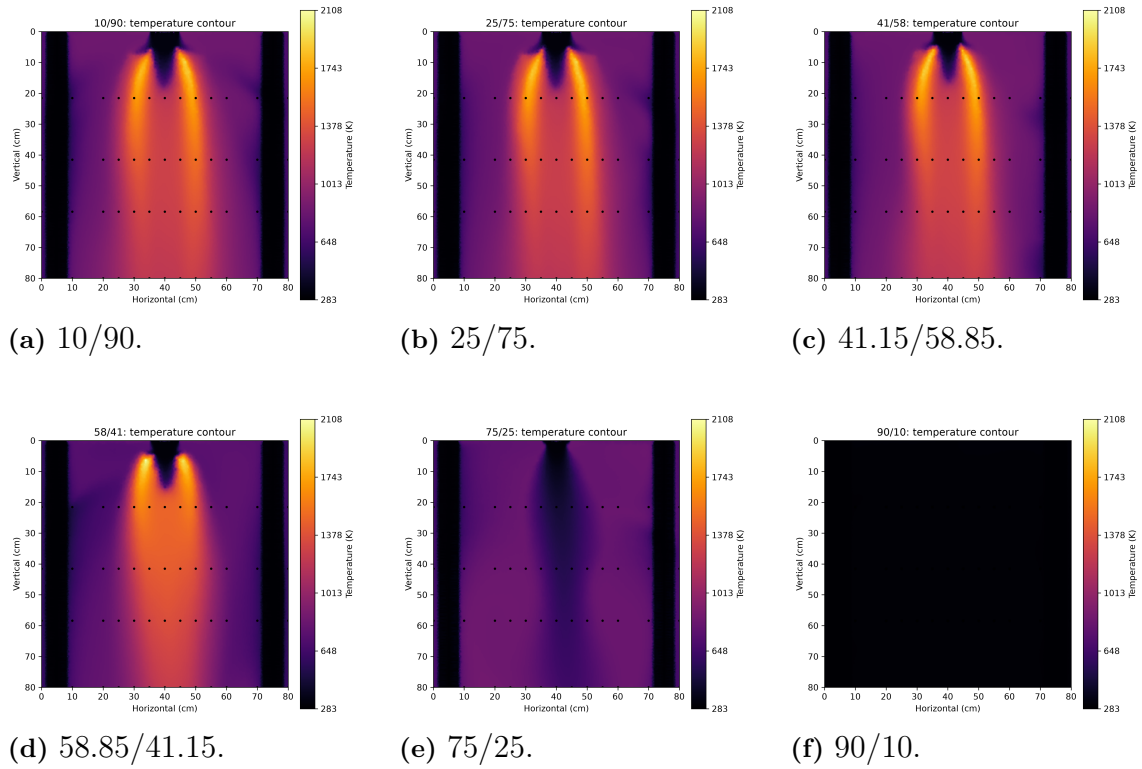


Figure D.1: Temperature contours for all air splits at $\lambda = 0.60$. The 75/25 and particularly 90/10 cases belong to different, weakly reacting or cold solution branches and should not be read as extensions of the four reacting rich cases.

D. Supplementary parametric-study images

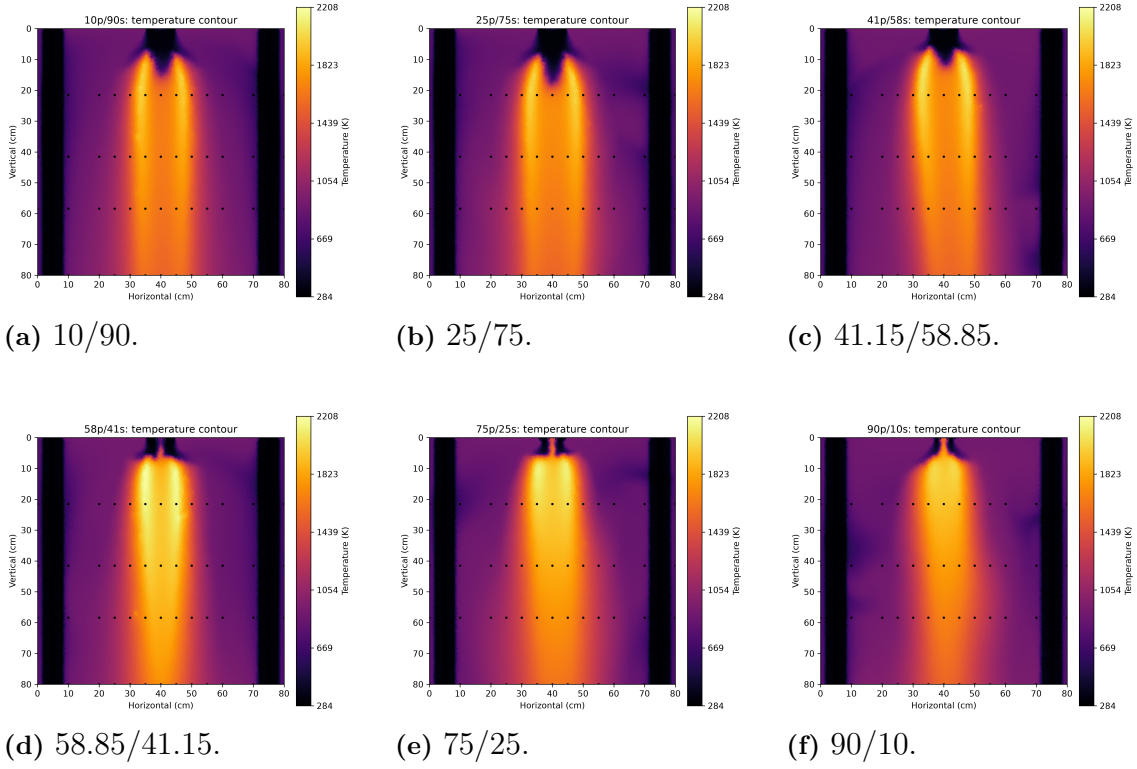


Figure D.2: Temperature contours for all air splits at $\lambda = 1.00$.

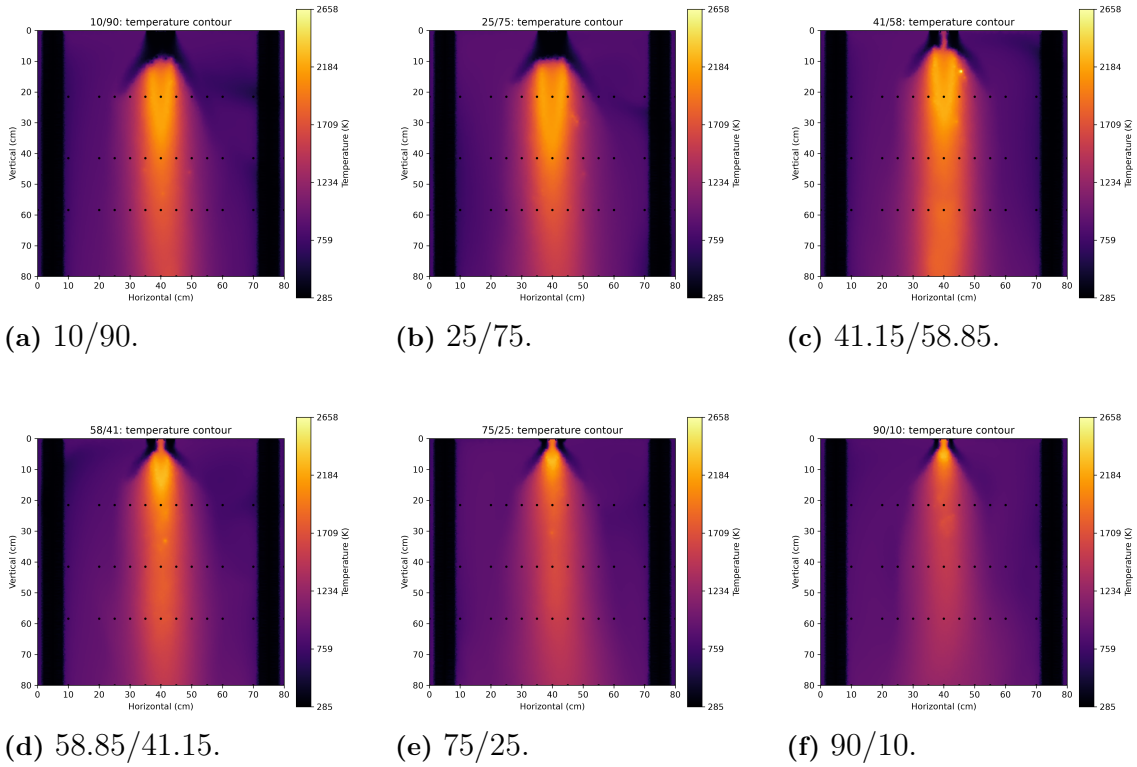


Figure D.3: Temperature contours for all air splits at $\lambda = 1.623$.

D.3 Infrared views not selected for the Results chapter

Figure D.4 completes the $\lambda = 1.00$ and 1.623 infrared-image sets. The 10/90, 41.15/58.85, and 90/10 views at these ratios were selected for the cross-ratio comparison in Results; the three intermediate splits below were omitted there to keep the comparison readable. All images use the common 0–15,000 $\text{W m}^{-2} \text{sr}^{-1}$ radiance scale used in the Results chapter.

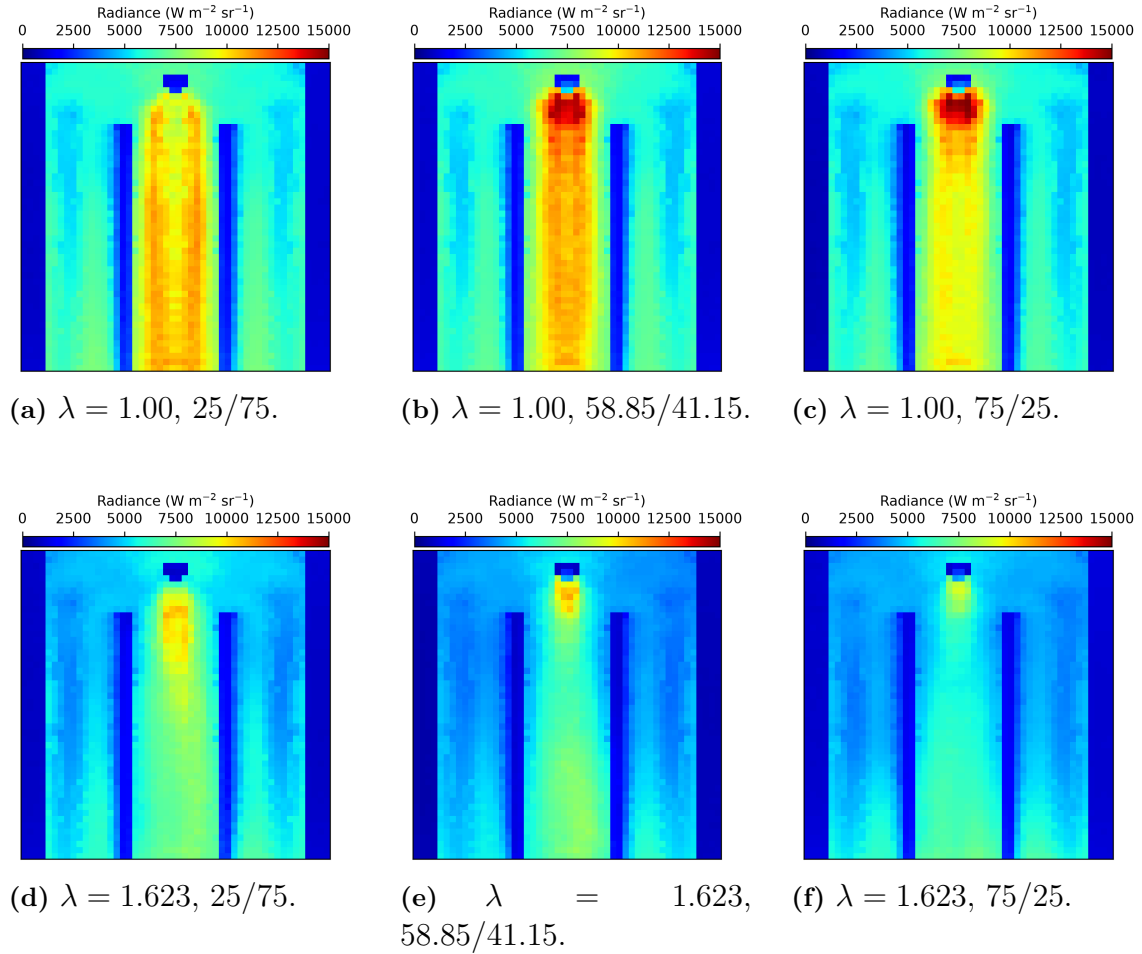


Figure D.4: Supplementary synthetic infrared images for the air splits not selected for the main cross-ratio comparison, shown on the common 0–15,000 $\text{W m}^{-2} \text{sr}^{-1}$ radiance scale.

E

Future work: exploratory machine-learning image-to-field reconstruction

This appendix preserves an exploratory study that is not part of the thesis aim, main results, or conclusions. It is included only as a documented direction for future work and should not be interpreted as a mature diagnostic method. The study used a proof-of-concept inverse model to estimate temperature, CO₂, and H₂O fields from one synthetic infrared image. The model complements the forward CFD–radiation calculation; it does not replace the Fluent solution or constitute validation against an independent physical infrared camera.

E.1 Literature basis for future inverse modelling

Inferring a combustion state from radiation is an inverse problem: the measured signal is known, while the temperature and composition fields that produced it are unknown. Ren et al. [32] trained multilayer perceptrons on synthetic infrared-emission spectra and retrieved non-uniform temperature and CO₂, H₂O, and CO concentration distributions. Their work combined a physics-based forward radiation model with a learned inverse mapping and showed that a model trained on synthetic radiation remains conditional on the spectral model and parameter range used to create its training data.

Bong et al. [33] combined a convolutional autoencoder with regressors to estimate total flow rate and equivalence ratio from monochrome images of a swirl combustor. Dai et al. [34] compared deep-learning architectures for reconstructing three-dimensional soot temperature and volume fraction from flame projections. These studies demonstrate the potential of image-based inference, but also its dependence on a sufficiently large and representative database.

The desired outputs in the exploratory study are spatial fields rather than single operating parameters. Principal component analysis (PCA), also known as proper orthogonal decomposition in many fluid-mechanics applications, represents correlated snapshots using a small number of orthogonal modes. Erichson et al. [35] compared modal reconstruction, ridge regression, and shallow neural networks for recovering fluid fields from limited sensors. Ridge regression adds an L_2 penalty to least squares and reduces variance caused by correlated predictors [36]. A U-Net encoder–decoder with skip connections [37] offers a more flexible image-to-image mapping, but the

26 independent training cases available here are insufficient for a defensible high-capacity convolutional model. This limitation motivates the reduced-order baseline described below.

E.2 Paired database and holdout design

The database contains 29 operating cases covering primary/secondary air split, excess-air ratio, propane mass-flow rate, and wall temperature. For every case, the input is the consistently rendered 1–5 μm radiation image and the targets are the corresponding Fluent temperature, CO_2 mole-fraction, and H_2O mole-fraction fields interpolated to a common 50×50 plane. The image is cropped to the common camera panel with the burner at the top and is represented by $50 \times 50 \times 3 = 7500$ RGB values.

Three complete cases were removed before model fitting: the $\lambda = 1.15$, 41/58 reference; the 1.5 g s^{-1} propane case; and the $\lambda = 1.623$, 58/41 case. The remaining 26 cases formed the training database. Excluding whole operating cases is essential: a random pixel split would place parts of the same CFD solution in both training and testing and would therefore not measure generalisation to an unseen flame state.

E.3 PCA–ridge architecture

Principal component analysis (PCA) compresses the correlated image pixels into a small set of image coefficients. A separate ridge-regression head maps those coefficients to compressed coefficients for each target. Inverse PCA then reconstructs three 50×50 fields. In compact form,

$$\mathbf{x}_{\text{IR}} \xrightarrow{\text{PCA}} \mathbf{z}_x \xrightarrow{\text{ridge head}} \mathbf{z}_{y,q} \xrightarrow{\text{inverse PCA}} \hat{\mathbf{y}}_q, \quad q \in \{T, X_{\text{CO}_2}, X_{\text{H}_2\text{O}}\}. \quad (\text{E.1})$$

Ridge regression determines coefficients $\boldsymbol{\beta}$ by

$$\underset{\boldsymbol{\beta}}{\text{minimise}} \|\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}\|_2^2 + \alpha\|\boldsymbol{\beta}\|_2^2, \quad (\text{E.2})$$

where α limits coefficient growth and reduces sensitivity to correlated image features. Independent output scaling prevents the temperature magnitude from dominating the species regressions.

A U-Net was considered as an image-to-image alternative, but was not used for the reported model. Only 26 statistically independent training cases were available, which is insufficient to support a high-capacity convolutional encoder–decoder without a serious risk of memorisation. Artificially flipped or recoloured copies would not create new combustion states and were therefore not counted as independent validation data.

E.4 Error measure

The percentage printed beneath each Fluent reference field is the relative mean absolute field error,

$$E_q = 100 \frac{N^{-1} \sum_{i=1}^N |\hat{y}_{q,i} - y_{q,i}|}{N^{-1} \sum_{i=1}^N |y_{q,i}|}, \quad (\text{E.3})$$

where $N = 2500$. This is not the mean of pointwise percentage errors, which would become unstable in cells where a reference concentration approaches zero. ML and Fluent panels use identical colour limits and the same virtual camera projection and four-rod geometry.

Table E.1: Relative mean absolute field errors for the three permanently excluded operating cases.

Excluded case	Temperature (%)	CO ₂ (%)	H ₂ O (%)
$\lambda = 1.15$, air split 41/58	6.07	12.90	6.95
Fuel rate 1.5 g s ⁻¹	6.45	11.95	5.68
$\lambda = 1.623$, air split 58/41	4.23	3.33	5.93

The temperature error remained between 4.23% and 6.45%, while H₂O remained between 5.68% and 6.95%. CO₂ was less uniform: its error was 3.33% for the $\lambda = 1.623$ case but approximately 12%–13% for the other two holdouts. In absolute terms, the CO₂ field mean absolute errors were 0.906, 0.927, and 0.215 percentage points, respectively. Thus, the large relative value partly reflects division by a mean CO₂ mole fraction of only about 0.07, but it also identifies CO₂ as the least robust output.

E.5 Held-out image comparisons

Figures E.1–E.3 show the input image, the three ML reconstructions, and the corresponding Fluent fields. The burner is at the top in every panel. The two central cooling rods and the two outer rods at the image boundaries are projected using the original infrared view rather than added as decorative overlays.

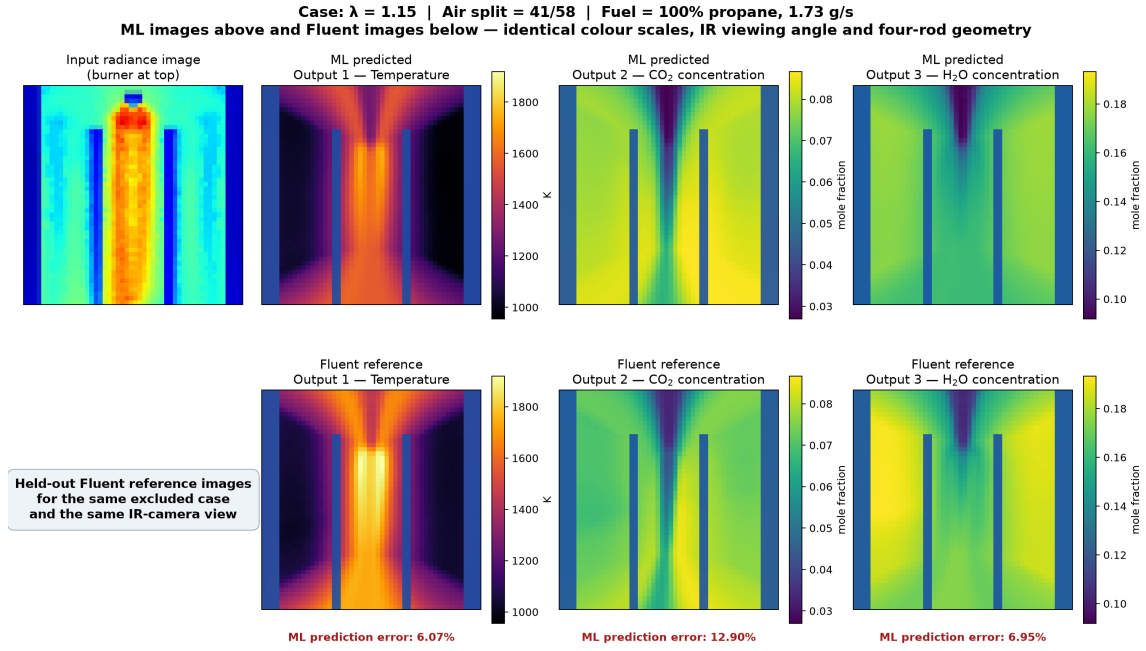


Figure E.1: Held-out $\lambda = 1.15$, 41/58 reference case. The upper row contains the infrared input and ML outputs; the lower row contains the corresponding Fluent reference fields.

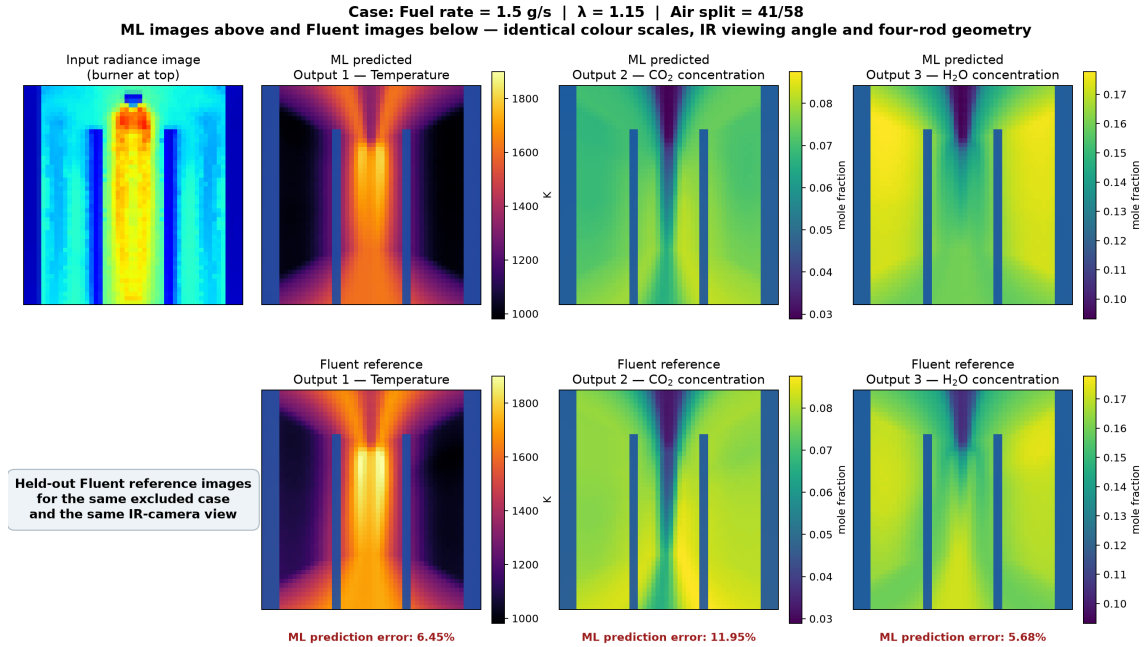


Figure E.2: Held-out 1.5 g s^{-1} propane-flow case, displayed with the same image-to-field comparison convention.

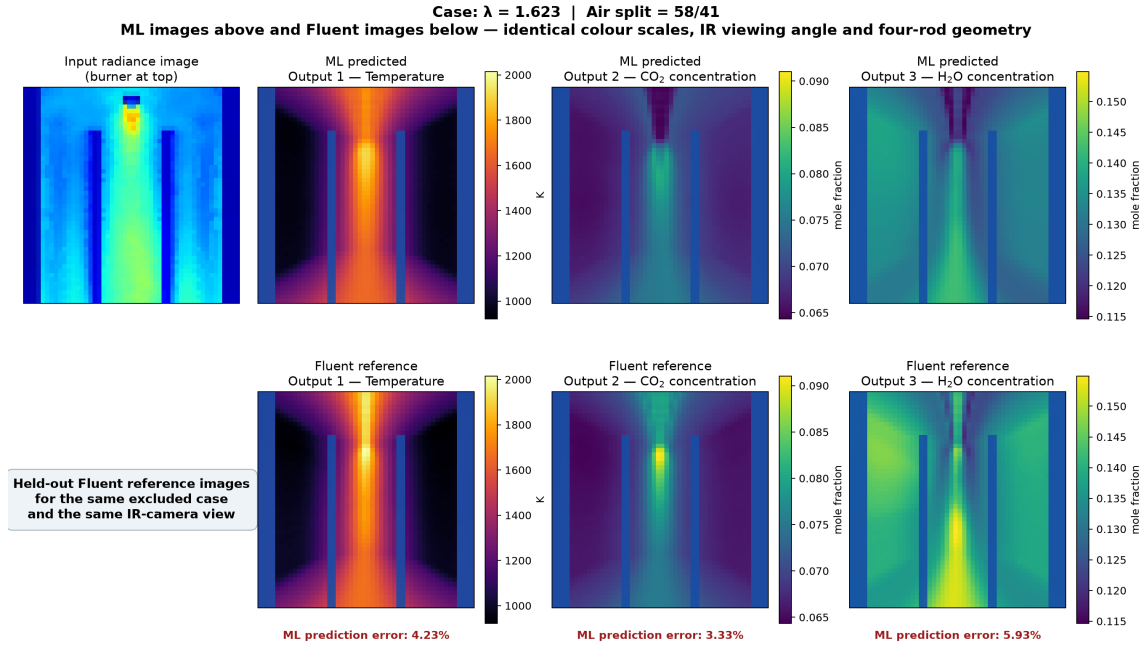


Figure E.3: Held-out $\lambda = 1.623$, 58/41 air-split case.

E.6 Interpretation and reproducibility

The holdout results show that the reduced-order mapping can recover the broad location and topology of the Fluent fields from an unseen synthetic image. They do not establish uniqueness of the inverse radiation problem: different three-dimensional states can produce similar line-of-sight intensities. The current input is also a colour-rendered PNG rather than the original numerical radiance array. Colour quantisation, resizing, and interpolation discard information before training. Future datasets should save the numerical radiance at each camera pixel together with its spectral and calibration metadata.

Each prediction run creates a new timestamped directory and identifies the operating case in both the directory and file names. The directory contains a PNG comparison, an NPZ archive of the three predicted numerical fields, and a JSON summary. Automatic comparison with Fluent is available for the three permanent holdouts. Application to a new experimental image would additionally require the same camera response, radiance calibration, spectral range, viewing angle, burner orientation, and rod geometry used in training.

F

Jones–Lindstedt reaction-rate user-defined function

The following C source is the user-defined function (UDF) used to supply the Jones–Lindstedt global reaction rates to ANSYS Fluent. The listing is reproduced verbatim from the simulation source file `j1_mech.c`. Species indices in the UDF must correspond to the mixture-species order stated in the code and configured in Fluent.

Listing F.1: Fluent UDF implementing the Jones–Lindstedt global reaction-rate mechanism.

```

1  #include "udf.h"
2  #include "math.h"
3  #include "string.h"
4
5  /* -----
6   Jones-Lindstedt (JL) global mechanism for C3H8 combustion.
7   Reversible steps split into irreversible forward/back pairs:
8   reaction-1 : C3H8 + O2 -> CO + H2      (fuel oxidation)
9   reaction-2 : C3H8 + H2O -> CO + H2      (fuel + steam)
10  reaction-3 : H2 + 0.5 O2 -> H2O          (H2 oxidation, fwd)
11  reaction-4 : H2O -> H2 + 0.5 O2         (H2 oxidation, rev)
12  reaction-5 : CO + H2O -> CO2 + H2       (water-gas shift, fwd)
13  reaction-6 : CO2 + H2 -> CO + H2O       (water-gas shift, rev)
14
15  The returned molar rate (rr) is integrated by the EDC
16  fine-structure reactor. The goals of this version are:
17  - smooth, single-valued rate surface -> ISAT can tabulate
18  - non-negative, finite rates          -> reactor integrates cleanly
19  - Arrhenius T clamped to a physical window -> no high-T runaway
20  - positive-order terms vanish at zero reactant -> no spurious heat
21  ----- */
22
23  #define GAS_CONST      8314.0      /* J/(kmol-K) */
24
25  /* Negligible guard, only to keep pow() finite on positive-order
26   terms. Must stay far below flame molar density (~1e-2 kmol/m3)
27   so reactions genuinely switch off where a reactant is absent. */
28  #define EPS_GUARD      1.0e-12
29
30  /* Larger floor used ONLY for reaction-4's NEGATIVE H2 order, to
31   bound its magnitude and move the kink into a region where H2 is
32   truly negligible. Tune in 1e-4 .. 1e-3 kmol/m3. */
33  #define H2_REV_FLOOR   1.0e-4
34
35  /* Temperature window for the Arrhenius factor. A numerical
36   overshoot in a cell cannot then drive the rate (and heat
37   release) super-physically high. Does not change normal kinetics. */
38  #define T_ARR_MIN      300.0
39  #define T_ARR_MAX      2500.0
40
41  /* Generous hard ceiling on the returned molar rate (kmol/m3/s).
42   Only clips pathological integrator excursions; set high enough
43   not to touch real combustion. Raise/lower or disable as needed. */

```

```

44 #define RATE_CEILING 1.0e6
45
46 /* Smooth, non-negative power law with a linear extension below Cmin.
47 - C <= 0      -> 0          (never pow(negative, fractional))
48 - C >= Cmin   -> pow(C, n)
49 - 0 < C < Cmin -> pow(Cmin, n-1) * C (continuous at Cmin) */
50 static real linearized_pow(real C, real exponent, real Cmin)
51 {
52     if (C <= 0.0) return 0.0;
53     if (C >= Cmin) return pow(C, exponent);
54     return pow(Cmin, exponent - 1.0) * C;
55 }
56
57 DEFINE_VR_RATE(jl_mech, c, t, r, mw, yi, rr, rr_t)
58 {
59     real T, T_arr, rho;
60     real c_C3H8, c_O2, c_CO2, c_CO, c_H2O, c_H2;
61     real kf = 0.0, rate = 0.0;
62
63     T = C_T(c, t);
64     rho = C_R(c, t);
65
66     /* Bail out cleanly on non-physical cell states */
67     if (T <= 0.0 || rho <= 0.0)
68     {
69         *rr = 0.0; *rr_t = 0.0;
70         return;
71     }
72
73     /* Arrhenius sees a clamped temperature */
74     T_arr = MAX(T_ARR_MIN, MIN(T, T_ARR_MAX));
75
76     /* Molar concentrations (kmol/m3).
77     Indices must match the Fluent mixture species order:
78     0:C3H8 1:O2 2:CO2 3:CO 4:H2O 5:H2 -- verify in Materials. */
79     c_C3H8 = rho * yi[0] / mw[0];
80     c_O2 = rho * yi[1] / mw[1];
81     c_CO2 = rho * yi[2] / mw[2];
82     c_CO = rho * yi[3] / mw[3];
83     c_H2O = rho * yi[4] / mw[4];
84     c_H2 = rho * yi[5] / mw[5];
85
86     if (strcmp(r->name, "reaction-1") == 0)
87     {
88         kf = 4.0e11 * exp(-1.2552e8 / (GAS_CONST * T_arr));
89         rate = kf * linearized_pow(c_C3H8, 0.5, EPS_GUARD)
90             * linearized_pow(c_O2, 1.25, EPS_GUARD);
91     }
92     else if (strcmp(r->name, "reaction-2") == 0)
93     {
94         kf = 3.0e8 * exp(-1.2552e8 / (GAS_CONST * T_arr));
95         rate = kf * linearized_pow(c_C3H8, 1.0, EPS_GUARD)
96             * linearized_pow(c_H2O, 1.0, EPS_GUARD);
97     }
98     else if (strcmp(r->name, "reaction-3") == 0)
99     {
100         kf = 8.5e15 * pow(T_arr, -1.0) * exp(-1.6736e8 / (GAS_CONST * T_arr));
101         rate = kf * linearized_pow(c_H2, 0.25, EPS_GUARD)
102             * linearized_pow(c_O2, 1.5, EPS_GUARD);
103     }
104     else if (strcmp(r->name, "reaction-4") == 0)
105     {
106         kf = 2.52e19 * pow(T_arr, -1.5) * exp(-4.149e8 / (GAS_CONST * T_arr));
107         rate = kf * linearized_pow(c_H2, -0.75, H2_REV_FLOOR) /* neg order */
108             * linearized_pow(c_O2, 1.0, EPS_GUARD)
109             * linearized_pow(c_H2O, 1.0, EPS_GUARD);
110     }
111     else if (strcmp(r->name, "reaction-5") == 0)
112     {
113         kf = 2.75e9 * exp(-8.368e7 / (GAS_CONST * T_arr));

```

```
114     rate = kf * linearized_pow(c_CO, 1.0, EPS_GUARD)
115           * linearized_pow(c_H2O, 1.0, EPS_GUARD);
116 }
117 else if (strcmp(r->name, "reaction-6") == 0)
118 {
119     kf = 9.268e10 * exp(-1.176e8 / (GAS_CONST * T_arr));
120     rate = kf * linearized_pow(c_CO2, 1.0, EPS_GUARD)
121           * linearized_pow(c_H2, 1.0, EPS_GUARD);
122 }
123 else
124 {
125     *rr = 0.0; *rr_t = 0.0;
126     return;
127 }
128
129 /* Keep the rate non-negative, finite and bounded */
130 if (rate < 0.0) rate = 0.0;
131 if (rate > RATE_CEILING) rate = RATE_CEILING;
132
133 *rr = rate;
134 *rr_t = rate; /* EDC integrates rr; rr_t mirrored as a safe default */
135 }
```

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