Numerical Modeling of Non-adiabatic Heat-Recirculating Combustors

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ABSTRACT

A two-dimensional numerical model of spiral counterflow heat recirculating combustors was developed including the effects of temperature-dependent gas and solid properties, viscous flow, surface-to-surface radiative heat transfer, heat conduction within the solid structure, one-step chemical reaction and heat loss from the combustor to its surroundings. A simplified model of heat loss in the 3rd dimension was implemented and found to provide satisfactory representation of such losses at greatly reduced computational cost compared to fully three-dimensional models. The model predicts broad reaction zones with structure decidedly different from conventional premixed flames. Extinction limits were determined over a wide range of Reynolds numbers (2 <Re < 5000) for propane-air mixtures. These limits showed reasonable quantitative agreement with experiments. Comparison of steady and unsteady calculations suggests there are no stability limits apart from these extinction limits. At Re > 500, modeling of turbulent flow and transport was required to obtain such agreement. Heat conduction along the heat exchanger wall has a major impact extinction limits; the wall thermal conductivity providing the broadest limits is actually less than that of air. Radiative heat transfer between walls was found to have an effect similar to that of heat conduction along the wall. In addition to weak-burning extinction limits, strong-burning limits in which the reaction zone moves out of the combustor center toward the inlet were also predicted by the numerical model, in agreement with experiments. It is concluded that several physical processes including radiative transfer, turbulence and wall heat conduction strongly affect the performance of heat-recirculating combustors, but the relative importance of such effects is strongly dependent on Re.

INTRODUCTION

It is well known that hydrocarbon fuels contain ≈ 100 times more energy per unit mass than lithium-ion batteries, thus devices converting fuel to electricity at >1%efficiency represent improvements over batteries for portable electronic devices [1]. At small scales, however, heat and friction losses become more significant, thus fuel-to-electricity conversion devices based on existing macro-scale designs such as internal combustion engines may be impractical. Consequently, many groups have considered heat-recirculating or "excess enthalpy" combustors for thermal management and thermoelectric, piezoelectric or pyroelectric devices, having no moving parts, for power generation. In heat-recirculating combustors, by transferring thermal energy from combustion products to reactants without mass transfer (thus reactant dilution), the total reactant enthalpy (sum of thermal and chemical enthalpy) can be higher than in the incoming cold reactants and therefore can sustain combustion under conditions (lean mixtures, low heating value fuels, large heat losses) that would extinguish without One such device is the spiral-wound counter-current "Swiss-roll" recirculation. heat-recirculating combustor [2-4] which provides large ratios of (internal) heat exchange area to (external) heat loss area. Some investigators [5-7] have studied straight-channel combustors without counterflow, in which streamwise heat conduction along the channel wall is the only means to recycle heat. This configuration is fundamentally different from counter-current combustors that rely primarily on conduction across the wall dividing from products to reactants for which streamwise conduction is almost always detrimental; consequently the performance of counter-current heat-recirculating combustors exceeds straight-channel combustors [5].

Experiments performed with properly instrumented macroscale devices are useful for predicting the performance of their microscale counterparts via correlations of dimensionless groups such as Reynolds number (Re), defined for this work based on the

inlet bulk velocity, channel width and kinematic viscosity at ambient conditions. (Note that Re decreases towards the combustor center as temperature (T) increases because the kinematic viscosity increases as T^{1.75} whereas velocity increases only as T¹ through the density effect {mass conservation requires density x velocity = constant}). However, because of the difficulties of fabricating, instrumenting and testing multiple combustor designs, Computational Fluid Dynamics (CFD) simulations are valuable design tools. Nevertheless, relatively few analytical/computational studies of heat-recirculating counter-current combustors have been performed. Jones et al. [4] performed global energy balances on reactant and product streams in counter-current heat-recirculating combustors using empirically-specified minimum reaction temperatures and heat losses. Two extinction limits were predicted: blow-off limits at large Re and heat loss induced limits at small Re, consistent with experiments [2, 3, 8]. Ronney [5] developed a predictive model of linear heat-recirculating combustors using overall heat transfer and heat loss coefficients (rather than specified heat loss [4]), thermally-thin heat conduction along the wall dividing reactant and product streams, and Arrhenius chemistry. Streamwise conduction along the channel wall was shown to exacerbate extinction greatly, particularly at low Re. Chen and Buckmaster [9] modeled Swiss-roll combustors "unwrapped" into straight channels assuming Poiseuille velocity profiles to avoid solving the momentum equation. Heat loss in the out-of-plane dimension was modeled with constant Nusselt number (whose value was not reported). Their results confirmed the role of streamwise conduction [5].

Swiss-roll experiments [8] also reveal "out-of-center" or "flashback" limits with respect to the spiral center (though reaction is still contained within the heat exchanger channels) but unlike conventional flashback limits, this limit occurs at sufficiently large, not small, flow velocities. No modeling study has explained this limit despite its practical importance (since it represents another bound on acceptable operating

parameters.) Moreover, all models show increasing fuel concentration at the extinction limit for larger Re (>500) that is not nearly as pronounced in experiments. This Re value corresponds roughly to transition to turbulence in plane channels, thus evaluation of turbulence effects in heat-recirculating reactors, not covered in any previous study, is warranted.

Consequently, our objective is to develop a CFD model of Swiss-roll combustors and compare its predictions to experiments (especially extinction and "out-of-center" limits) over wide Re ranges. Such models may prove useful to the design of both macroscale and microscale combustors; in microscale devices instrumentation difficulties may render computations the only viable design tool. This study focuses on macroscale devices, however, it will be shown that proper calibration and verification at macroscales is an important prerequisite to successful modeling of microscale devices.

NUMERICAL MODEL

The Swiss-roll combustor geometry (Fig. 1) was chosen to match experiments [8] on propane-air combustion in a 3.5-turn square inconel spiral heat exchanger with an open central region. The channel width, wall thickness and overall dimensions are 3.6 mm, 0.5 mm and 70 x 70 mm, respectively. The conservation equations of mass, chemical species, momentum and energy were solved for two-dimensional (x-y plane) steady low Mach number viscous flow, heat transfer and chemical reaction using the FLUENT 6.1 CFD package. An optimized nonuniform grid with 20877/3158 cells in the gas/solid phase was employed. Grid-independence of the results was verified. The combustor height (in the z-direction) is incorporated via specification of heat loss coefficients described below. Since preliminary studies [10] showed that radiative transfer within the heat exchanger is important, surface-to-surface radiation was modeled via Discrete Ordinates with inconel wall emissivity 0.35 [11]. Simple estimates show that for the path-lengths and species partial pressures of interest, gas-phase radiative transfer is negligible compared to convection and surface-to-surface radiation. All gas- and thermodynamic and transport modeled solid-phase properties are as temperature-dependent using handbook values. Turbulent flow and heat transfer is modeled using the standard k- ε model. While probably no statistical turbulence model accurate at the transitional Reynolds numbers (≤5000) studied here, the k-ε model is nevertheless considered useful for semi-quantitative evaluation of turbulence effects. A far more computationally intensive Direct Numerical Simulation would probably be required for more accurate results.

Propane-air reaction was modeled using a one-step mechanism. The activation energy (30 kcal/mole) and fuel/oxidant concentration coefficients (0.1/1.65) were taken from [12], but since this mechanism was developed for propagating flames, it is not directly applicable for low-temperature, broad reaction zone structures in Swiss-roll combustors. Consequently, the reaction rate pre-exponential factor (1.8x10⁷ in kg-mole, m³, sec units) was chosen to obtain the same extinction limit as in experiments [8] for Re=1000. This large Re was chosen because, as our results show, heat loss, wall conductivity and radiative transfer are unimportant at this condition, thus any inaccuracies in these sub-models will not affect the choice of pre-exponential factor. *The same pre-exponential factor was used for all computations and no other adjustable parameters were employed*.

Heat loss in the z-direction is modeled via a volumetric sink term (Q_{loss}) in the energy equation that matches the experimental configuration as closely as possible. Q_{loss} simulates conduction (in the solid-phase) or convection (in the gas-phase) to insulating blankets and aluminum plates on the top/bottom of the Swiss-roll, conduction through the blankets/plates, and natural convection and radiation to ambient air:

$$Q_{loss,s} = -\frac{2}{H} \frac{\left(T_c - T_{\infty}\right)}{\sum R_{th,s}}; Q_{loss,g} = -\frac{2}{H} \frac{\left(T_c - T_{\infty}\right)}{\sum R_{th,g}}$$
(1)

$$\sum R_{th,s} = \frac{H}{2\lambda_s} + \frac{\tau_b}{\lambda_b} + \frac{\tau_{Al}}{\lambda_{Al}} + \frac{1}{h_{\infty}}$$
(2)

$$\sum R_{th,g} = \frac{1}{h_{g,z}} + \frac{\tau_b}{\lambda_b} + \frac{\tau_{Al}}{\lambda_{Al}} + \frac{1}{h_{\infty}}$$
(3)

Here H is Swiss-roll combustor height, T_c the (modeled) temperature inside the combustor, T_{∞} ambient temperature, $R_{th,g}/R_{th,s}$ total thermal resistance through the gas/solid-phase paths, λ_s combustor wall thermal conductivity, τ_b top/bottom insulating blanket thickness, λ_b its thermal conductivity, τ_{Al} top/bottom aluminum plate thickness, λ_{Al} thermal conductivity, \mathbf{h}_{∞} effective (temperature-dependent) heat transfer coefficient from the top/bottom plates to ambient due to combined buoyant convection (10 W/m²°C) and radiative heat transfer (Al plate emissivity 0.25), and $\mathbf{h}_{g,z}$ heat transfer coefficient from the reactive gas mixture to the insulating blankets in the z-direction.

The inlet boundary condition is a specified plug-flow velocity with ambient (300K) temperature reactants. The outlet condition is ambient pressure. The combustor external surfaces (in the x-y plane) experience heat loss via natural convection with heat transfer coefficient $10 \text{ W/m}^{2\circ}$ C and radiative transfer with inconel wall emissivity 0.35.

Computations were started with mixtures away from extinction limits. The initial conditions were high (\approx 1000K) center temperatures tapering to ambient at the outer boundary. This was sufficient to "ignite" reaction and converge to steady solutions. Converged solutions were used as initial conditions for subsequent computations in which the inlet composition or velocity was changed slightly, then new converged solutions were obtained. This process was repeated until extinction was observed, in which case the center temperature would decrease continuously to ambient during the iterations. As in experiments [8], this extinction process was found to be abrupt and well-defined. As might be expected from one-step chemistry, fuel leakage through the

reaction zone was insignificant even at the lean extinction limits; this is consistent with experimental observations [8].

A rigorous stability analysis is beyond the scope of this work, but simple tests was performed using converged, steady solutions as initial conditions to FLUENT's unsteady solver. Many conditions were studied both in the centered-reaction and out-of-center regimes, but *in no case did a steady solution diverge*. Consequently, the solutions reported here are probably stable (at least to small disturbances), physically observable results.

RESULTS

Effects of turbulence

Figure 2 shows extinction limits for the complete model and that with laminar flow (turbulent flow and transport artificially suppressed). In both cases, at some fixed values of fuel concentration (for example 1.5%), there are both low-Re heat loss induced limits and high-Re "blow-off" limits, consistent with prior studies. The predicted extinction limits at high Re are significantly extended with turbulence. This is because turbulence increases heat transfer to/from the heat exchanger dividing wall. For heat-recirculating combustors, the adiabatic reactor temperature T_r is, in dimensional form (see [5], Eq. 16)

$$T_r = T_{ad} + \frac{h_g L Y_{f,\infty} Q_R}{2\dot{m} C_P^2}$$
(4)

where T_{ad} is the adiabatic combustion temperature (without heat recirculation), h_g heat transfer coefficient to/from the dividing wall (in the x-y plane), L wall length, $Y_{f,\infty}$ inlet fuel mass fraction, Q_R fuel heating value, \dot{m} mass flow per unit depth in the z-direction and C_P specific heat. For laminar flow h_g is constant (independent of flow velocity and thus \dot{m}) thus the excess enthalpy $C_P(T_r-T_{ad}) \sim \dot{m}^{-1} \sim Re^{-1}$ whereas for turbulent flow, roughly $h_g \sim \dot{m}$, thus $C_P(T_r-T_{ad}) \approx constant$. Even at Re=1000, at the extinction limits h_g (averaged over all interior walls) is 1.41x higher and $Y_{f,\infty}$ 1.55x lower with turbulence included. Therefore, when turbulent transport is present T_r will be larger and chemical reaction faster, thus more resistant to extinction at the high-Re, residence time limited "blow-off" limit. Consequently, *even though no turbulence occurs in low-Re microscale combustors, inclusion of turbulence effects in models of scaled-up devices is necessary for proper calibration and validation of models with experiments* (for example via the pre-exponential factor.)

As expected, at low Re the turbulent- and laminar-flow models converge. Self-sustaining combustion cannot occur at Re<40, even for stoichiometric mixtures, which is close to the experimental value of 36. *This agreement was obtained with no adjustable parameters other than the reaction rate pre-exponential factor, which was adjusted for conditions where heat loss is unimportant.* Consequently, the heat transfer and loss models employed here are considered realistic and appropriate. Moreover, between the "anchor point" at Re=1000 and the low-Re limit, the computed and measured extinction limits track each other reasonably well, though computed limits are slightly lower.

To compare measured and predicted temperatures systematically, seven "virtual thermocouple" stations were created (Fig. 1, labels TC1-TC7), each 1 mm by 1 mm, at the same locations as in experiments [8], and computed temperatures averaged over each virtual thermocouple region. (These temperatures are not the maxima determined on a cell-by-cell basis over the entire computational domain but provide the most realistic comparison between model and experiment.) For both simulations and experiments, for all Re the maximum thermocouple temperature (T_{max}) was always at TC1 for mixtures sufficiently close to extinction limits. Figure 3 shows that the effect of Re on limit temperature shows the same trend in model and experiment, though experimental values are systematically lower. This is typical of one-step chemical models without chain branching reaction steps [12]. Figure 3 also shows that at low Re, despite heat recirculation the peak temperatures are less than T_{ad} due to heat losses, whereas for higher Re (above ≈ 100) where heat loss is less important, this trend is reversed. An interesting

feature of Figure 3 is that *limit temperatures with and without turbulent transport are nearly identical even though the limit* T_{ad} and mixture strengths (Fig. 2) are different. This is likely because (as will be shown later) at high-Re conditions where turbulent flow is present, extinction is caused by insufficient residence time in the combustor center (where temperature is highest) compared to the reaction time scale, rather than heat losses. This residence time is set by the flow velocity (thus Re). Consequently, Re sets the chemical reaction rate required to avoid extinction, which is far more sensitive to temperature than any other property. Thus, a given Re requires a given reaction temperature to avoid extinction, regardless of the transport environment required to obtain this temperature. In most combustors, chemistry-turbulence interactions would greatly complicate this explanation, but (as shown later) reaction zones in Swiss-roll combustors are much broader than the channel width and thus the largest turbulence scales, hence substantial chemistry-turbulence interactions are not expected.

Heat-recirculating combustors transfer energy from combustion products to reactants and thereby increasing the total enthalpy of the reactants. Therefore, heat transfer and excess enthalpy should be related. The total heat recirculation should be proportional to the difference between the temperature of each outlet turn (T_o) and each inlet turn (T_i) . With this motivation a dimensionless heat transfer parameter $Q=\Sigma(T_o-T_i)]/T_{\infty}$ was defined. (In principle the differing areas of each turn should be considered, but each successive turn inward is hotter, thus thermal conductivity is higher, which partially offsets the area effect.) Figure 4 shows the predicted correlation between Q and dimensionless excess enthalpy (H) defined as $(T_{max}-T_{ad})/(T_{ad}-T_{\infty})$ for all limit conditions. These predictions are in good agreement with experiments - even though T_{max} differs between model and experiment, the temperature differences between turns (T_o-T_i) , the resulting heat recirculation (Q) and its effect on T_{max} (via H) is reasonably represented by the current model.

Effects of heat loss and radiation

Figure 5 shows the effect of artificially suppressing surface-to-surface radiation within the combustor or convective/radiative heat losses from the combustor external surfaces (in both the x-y plane and the z-direction) to ambient. All 3 extinction curves exhibit the same dual-limit behavior but only the lower limit is affected by suppression of heat loss or radiation. Without heat loss / radiation the low-Re limit is 3 / 12 compared to 40 with both effects included. At high Re the reactant chemical enthalpy flux (thus heat release) greatly exceeds heat loss or heat transport via radiation, thus insufficient residence time compared to the chemical time scale (rather than losses) determine extinction conditions. At low Re, residence times are longer and the chemical enthalpy fluxes are smaller, thus heat losses dominate extinction [4-7]. <u>Both</u> heat losses and surface-to-surface radiation significantly affect low-Re extinction limits, and suppression of either causes disagreement between model and experiment, again indicating that the heat loss and radiation models employed are appropriate.

It is interesting that suppressing surface-to-surface radiation has an effect similar to suppressing heat loss. In fact, for 50 < Re < 500, extinction limits are actually wider with radiation excluded (but heat loss still included) than vice versa. *A priori* one might expect radiation to increase heat recirculation which would extend limits, however, heat recirculation requires heat transfer to the gas. Since the gases are essentially transparent on the channel width scale, the gases would absorb/transmit very little radiation (even if gas radiation were included in the model). Consequently, radiation transfers heat directly between walls rather than to/from the gases, and thus has qualitatively similar effect to streamwise heat conduction along the wall, which (as quantified later) is very detrimental to combustor performance [5].

Since conductive transfer through the gas with conductivity $\lambda_{\rm g}$ between walls

separated by a distance w scales with $\lambda_g(T_i - T_o)/w$, whereas radiative transfer scales as $\sigma \epsilon(T_i^4 - T_o^4)$, the ratio of conductive to radiative transfer is proportional 1/w. Thus, the importance of radiation diminishes as scale (w) decreases, but (as with turbulence) radiation must be included in macroscale models to ensure proper validation and calibration of models intended for simulation of microscale devices.

Effect of wall thermal conductivity

Heat-recirculating combustors require dividing walls between reactants and products to enable transfer of thermal enthalpy from products to reactants without product mass recirculation. Prior studies [5, 9] showed that streamwise heat conduction along the wall is detrimental to performance, however, for zero wall thermal conductivity, no heat recirculation is possible, thus, an optimum conductivity causing the widest possible extinction limits must exist. (This behavior was not predicted in [5, 9] because thermally-thin heat exchanger walls were assumed *a priori*.)

Figure 6 shows the effect of wall thermal conductivity on extinction limits for Re=50. The optimum conductivity is extremely small – in fact, smaller than air. Consequently, for any solid material from which heat exchanger walls may be constructed, lower thermal conductivity is always advantageous.

The following estimate of this optimum is proposed. There is no disadvantage to lower wall conductivity until the wall thermal resistance $\sim \tau/\lambda_s$ is comparable to the thermal resistance between gas and wall $\sim 1/h_g$. At higher λ_s , streamwise wall conduction reduces performance, whereas at lower λ_s heat recirculation via conduction across the wall is diminished. Thus at the optimum condition $\lambda_s \approx h_g \tau \approx (10.6 \text{ W/m}^2\text{K})(0.0005 \text{ mm}) = 0.0056 \text{ W/mK}$ (here h_g is averaged over all interior walls), which is comparable to the calculated optimal value (Fig. 6).

Out-of-center limits

For sufficiently strong mixtures away from extinction limits, reaction can be sustained without the full benefit of heat recirculation (thus higher temperatures) that exists at the combustor center. In this case the location of peak reaction rate shifts towards the inlet. Figure 7 illustrates this point for Re=500. Near the extinction limit (1.0% propane) the reaction zone is centered, but (as experiments [8] confirm) shifts toward the inlet for stronger mixtures. For 2.8% propane this peak shifts 2 full turns toward the inlet. If Fig. 7 is replotted (not shown) with reaction rate scaled by ambient fuel concentration and position shifted by location of maximum reaction rate, all these curves are nearly identical. Note that the reaction zone half-width at half the peak reaction rate is 10-15 cm, which is far greater than any conventional propagating flame thickness. Thus, as experiments [8] confirm, it is more appropriate to consider reaction in heat-recirculating combustors as "mild" or "flameless" combustion [13, 14].

Non-centered reaction zones cause reversals of temperature gradients that are problematic for thermoelectric and other power conversion devices. Consequently, only the band of conditions between extinction and "out-of-center" limits may represent viable operating conditions for practical devices. Figure 8 shows predicted and measured out-of-center limits, defined as conditions where the maximum real or virtual thermocouple temperature occurs at TC3-TC7 (not TC1 or TC2). The agreement is reasonable considering that single-step chemistry is employed and nothing was adjusted to obtain this agreement (the pre-exponential factor was adjusted to match extinction, not the out-of-center limit), though, as with extinction limits, the predicted out-of-center limits are somewhat lower than experimental values. As with extinction limits, turbulent flow and transport modeling provides significantly better agreement with experiments at high Re.

While the "out-of-center" limit is a "flashback" limit (reaction zone moving

upstream) with respect to the combustor center, unlike conventional flashback limits it occurs at sufficiently high (not low) Re. As shown above, the low-Re limits are due to heat losses and thus for fixed fuel concentration, heat loss is less dominant as Re increases, thus the ratio of heat generation to loss (and consequently peak temperature) increases. Since reaction time decreases exponentially with temperature, as Re increases the reaction time can decrease faster than residence time (proportional to Re) increases, thus causing the reaction zone to move toward the inlet where less heat recirculation occurs, temperature decreases and thus reaction time increases until it is balanced by residence time. Consequently, the combined effect of heat recirculation and loss cause out-of-center (flashback) limits near low-Re limits to behave differently than in conventional combustors.

CONCLUSIONS

Spiral counter-current heat-recirculating "Swiss-roll" combustors were studied over a three-decade range of Reynolds number using a simple two-dimensional CFD model including temperature dependent properties, turbulent flow and transport, surface-to-surface radiation, one-step chemical reaction and heat losses. By using steady solutions as initial conditions for transient calculations, it was determined that all steady solutions obtained were probably stable, at least to small disturbances. Agreement between predicted and measured extinction and out-of-center limits is reasonable across a large range of Re, especially considering the simplicity of the chemical and turbulence models employed. Radiation and heat loss effects are inconsequential at high Re but dominant at low Re, whereas at high Re turbulent transport modeling is essential to determine heat recirculation (thus limits) accurately.

Streamwise heat conduction along the wall diving reactant and product streams removes thermal enthalpy from the central reaction zone that is subsequently lost to ambient, thus reducing reaction temperatures and promoting extinction. Consequently, lowering wall conductivity greatly widens extinction limits. However, conduction across the wall is required for heat recirculation to occur, thus an optimum conductivity must exist. This optimum conductivity is shown to be smaller than air – an impractically small value. Thus, practical Swiss-roll combustors operating at low Re will always suffer degraded performance due to streamwise conduction. This suggests that plastics, whose conductivities are perhaps the lowest of dense (non-porous) solids, may be advantageous, at least in the outer turns where temperatures are compatible with high-temperature polymers ($\approx 500^{\circ}$ C).

Surface-to-surface radiation has detrimental effects analogous to increasing combustor wall thermal conductivity. Scaling arguments show that while radiative transfer may not be important compared to conduction/convection in microscale devices, they must be retained in models calibrated using macroscale experiments. Similar considerations apply to turbulence effects.

While reasonably accurate predictions were obtained using single-step chemistry, the predicted maximum temperatures at the extinction limit are than experimental values, which is typical result for single-step chemistry without chain branching steps. Future computations will include more detailed chemical mechanisms. Moreover, while the low-Re heat loss induced extinction limit was very well predicted by the two-dimensional model including out-of-plane heat loss modeled using a volumetric term, fully three-dimensional calculations may be required in practical combustors integrated with other components that complicate the description of out-of-plane losses.

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FIGURE CAPTIONS

Figure 1. Geometry and grid structure of the modeled Swiss-roll combustor.

Figure 2. Extinction limits obtained using the full model, with turbulent flow and transport suppressed, and comparison to experiments [8].

Figure 3. Maximum thermocouple temperatures and adiabatic combustion temperatures at extinction limits obtained using the full model, with turbulent flow and transport suppressed, and comparison to experiments [8].

Figure 4. Relationship of excess enthalpy (H) to heat transfer parameter (Q) obtained using the full model and comparison to experiments [8].

Figure 5. Extinction limit obtained using the full model, full model without radiation (heat loss included) and full model without heat loss (radiation included).

Figure 6. Effect of wall thermal conductivity on extinction limits for Re = 50.

Figure 7. Reaction rate along the channel center at Re = 500 for varying fuel concentration.

Figure 8. Out-of-center limits obtained using the full model, with turbulent flow and transport suppressed, and comparison to experiments [8].



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