simplification in calculating the physical particle distribution over a grid could mean substantial gains in code efficiency. Moreover, there will be virtually no accompanying increase in numerical noise generation as compared with predictions using normal pdfs. In some cases, it may also be acceptable to apply the theory with the even simpler uniform pdfs where rapid computation of an approximate solution is desired.

Acknowledgments

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References

[1]Litchford, R. J., and Jeng, S.-M., "Efficient Statistical Transport Model for Turbulent Particle Dispersion in Sprays," *AIAA Journal*, Vol. 29, No. 9, 1991, pp. 1443–1451.

[2]Litchford, R. J., and Jeng, S.-M., "Efficiency of a Statistical Transport Model for Turbulent Particle Dispersion," *AIAA Journal*, Vol. 30, No. 5, 1992, pp. 1434–1438.

Statistical Modeling of Turbulent Dilute Combusting Sprays

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Introduction

THIS Note comments on the application of a new statistical transport model for turbulent particle dispersion[1-3] to dilute combusting sprays. The approach taken was to examine model performance with respect to available experimental data. Comparison with predictions using a conventional direct modeling technique was also made. The particular test conditions for the experiment may be described as a dilute monodispersed spray of fuel droplets injected into a round, turbulent diffusion flame. Our primary interest in this work was to justify the use of the statistical transport model for combusting droplets and to demonstrate the potential for improved efficiency with minimal sacrifice in accuracy.

Approach

The fundamental data reported by Shuen et al.[4,5] proved very useful because of the simple test configuration of their experiments. The flow conditions produced may be well characterized by established theoretical methods allowing computation of the detailed flowfield. The physical conditions of their experiments are fully described in Ref. 5. Here we provide a brief summary of the test arrangement. Methane is vertically injected upward through a converging nozzle with a throat diameter of 5 mm. The exit Reynolds number is 1.17×10^4 with a centerline velocity of 52.8 m/s. The injection temperature is a nominal 300 K. The resulting fully turbulent diffusion flame burns in stagnant air at atmospheric pressure. A dilute monodisperse spray of methanol droplets was introduced with initial drop diameters of 105 and 180 μm. The spray injection rates are summarized in Table 1.

To evaluate the proposed dispersion model, numerical methods are used to compute the mean background flow for the turbulent diffusion flame. With the proper initial/boundary conditions known from measurements, the continuous-phase analysis may be performed and validated against flame structure data. The calibrated theoretical solution then provides the necessary flowfield resolution to evaluate dispersion models.

The theoretical methods of Jeng and Faeth[6] are employed for the continuous-phase analysis. For the dilute spray assumption, drop source terms in the continuous phase are ignored. Furthermore, boundary-layer approximations are applicable so that the governing flow equations become parabolic. Jeng and Faeth's method for analyzing this flow involves solution of a Favre-averaged formulation due to Bilger[7] with a κ-ϵ-g turbulence closure. By introducing a conserved-scalar (mixture fraction) formalism, the governing equations are solved for mean conservation of mass, momentum, and mixture fraction. Instantaneous scalar properties are then determined from the mixture fraction probability density functions (pdf) with appropriate state relationships.

Applying a two-parameter clipped Gaussian function for the Favre pdf, the mean and variance are computed from the known mixture fraction and square mixture fraction fluctuation as described by Lockwood and Naguib.[8] With the Favre pdf fully defined, Favre-averaged values of all scalar properties may then be computed. A relation also exists for obtaining time-averaged mean quantities. The necessary state relationships are constructed according to the laminar flamelet method of Bilger[9] and Liew et al.[10] This method is based on the observation that temperature and species concentrations in laminar diffusion flames are nearly unique functions of mixture fraction alone. Laminar flamelet correlations are then developed from laminar flame measurements and applied to turbulent diffusion flames. This is accomplished by viewing a turbulent flame as a sequence of laminar flamelets passing a given location in the flow. Jeng and Faeth[6] constructed the state relationship for methane burning with air from laminar flame measurements.

Our statistical treatment of turbulent sprays may be described as a stochastic-dispersion-width-transport (SDWT) model. It is based on coupling a direct modeling approach for particle/eddy interactions with continuous two-parameter probability density functions to describe the physical particle spatial and temporal distribution. In the current formulation, a computational parcel is represented by a normal pdf in space. The mean of each pdf is determined by Lagrangian tracking of each parcel through a sequence of stochastically generated turbulent eddies. The variance of each pdf is represented by a turbulence-induced mean square dispersion as determined from a statistical formulation based on the linearized particle equations of motion. Convolution of the parcel pdfs yields the probable physical particle distribution at a given instant in time. Full details of the theoretical formulation are available in previous publications.[1-3]

Like Shuen et al.,[4,5] we also examine the basic stochastic-separated-flow (SSF) direct modeling approach, which is recovered as a special case of the SDWT model by introducing a delta-function representation for each computational parcel.

Table 1 Spray injection rates

Nominal drop diameter, μm	105	180
Liquid volume flow rate, μl/s	12.21	24.48
Nominal injection rate, drops/s	20,000	8,000

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However, we do not bother to re-examine the deterministic-separated-flow (DSF) model where drop-turbulence interactions are ignored. Complete neglect of turbulence effects on the spray is known to drastically underestimate dispersion.

Following Shuen et al.,[4,5] a discrete droplet transport model is applied to estimate the vaporization characteristics of each parcel as a single representation for an entire particle group. Specifically, a quasisteady, gas-phase, diffusion-controlled transport formulation is employed with empirical correlations for forced convection and aerodynamic drag. The surface is assumed to be in thermodynamic equilibrium, binary diffusivities are considered equal for all species, and constant average transport properties are assumed at each instant in time. Based on the observations of Shuen et al.,[4,5] envelope flames are considered unimportant for the test conditions of interest and are therefore neglected. Under the dilute spray assumption, drop shattering and collisions are also neglected. In contrast to the thin-skin internal energy transport model applied by Shuen, however, we consider transient heating using the uniform drop temperature approximation. The drop life history calibrations of Shuen et al.[4,5] also provide the optimum weighting parameter to define the property reference state in the gas phase. Thermodynamic and thermophysical properties are evaluated as documented in Ref. 5.

In regard to turbulence effects on droplet vaporization characteristics, only relative velocity fluctuations are considered here. It is possible to randomly sample for the instantaneous mixture fraction fluctuations by converting the Favre-averaged pdf to a time-averaged pdf and thus obtain instantaneous scalar properties for each eddy using the known state relationships. But we chose to neglect scalar property fluctuations and use local mean values only. A comparison of our predictions with the results of Shuen et al.[4,5], which account for scalar property fluctuations, indicate that such considerations have little influence on the overall spray structure.

Results

Measurements 1 injector diameter downstream from the burner nozzle provided the necessary initial conditions for the continuous-phase analysis. These measurements included the mean streamwise velocity and the turbulent velocity fluctuations. The initial turbulent kinetic energy dissipation rate ϵ was estimated from the measured decay rate of the turbulent kinetic energy k and the mean streamwise velocity $\bar{u}$ as $\epsilon = -\bar{u}(dk/dx)$. The mean gas-phase injection temperature was a nominal 300 K. Since the gas injected through the burner nozzle was pure methane, we could also surmise that the initial mixture fraction is unity and the mean square mixture fraction fluctuation is zero by definition. This information provides complete specification for the continuous-phase analysis. Computed solutions of the parabolic Favre-averaged partial differential equations based on these conditions yielded satisfactory agreement with reported measurements.

For the dispersed phase, measured initial drop diameters, mean and fluctuating streamwise velocities, and fluctuating radial velocities were available as well as the initial drop number flux distributions. The measured initial drop diameters were reported as constant. The two cases considered were for $d_0 = 105$ and 180 μm. The initial mean streamwise drop velocities were also reported as 15.6 m/s for the 105 μm drops and 12.0 m/s for the 180 μm drops. For our computations, the droplets were injected with a nominal temperature of 300 K at the mean injection velocity. Initial drop velocity fluctuations were small and therefore neglected. The radial position at injection for each drop was determined by randomly sampling over

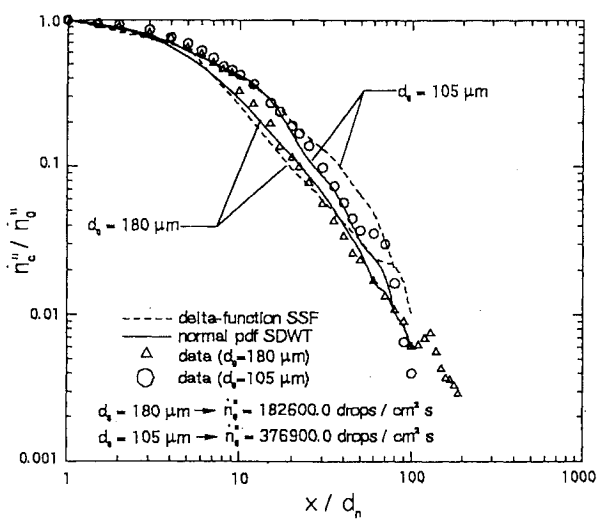

Fig. 1 Time-averaged drop number flux along flame axis.

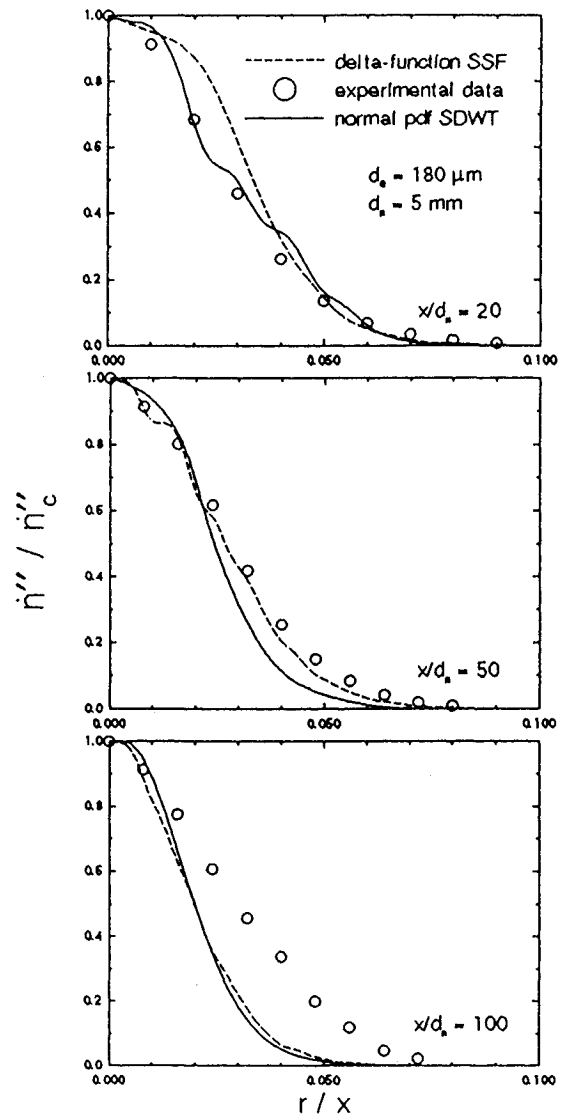

Fig. 2 Time-averaged drop number flux radial profiles ($d_0 = 180$ μm).

Table 2 Spray modeling parameters

Model	SSF		SDWT	
d_0, μm	105	180	105	180
N_{pp}	20,000	8000	20,000	8000
N_{pp}/N_{cp}	1	1	200	200
$N_{cp}^{(e)}$	1	1	2	2
Δt_{samp}	0.5	1.0	0.5	1.0
$N_{cp_{samp}}$	10,000	8000	50	40

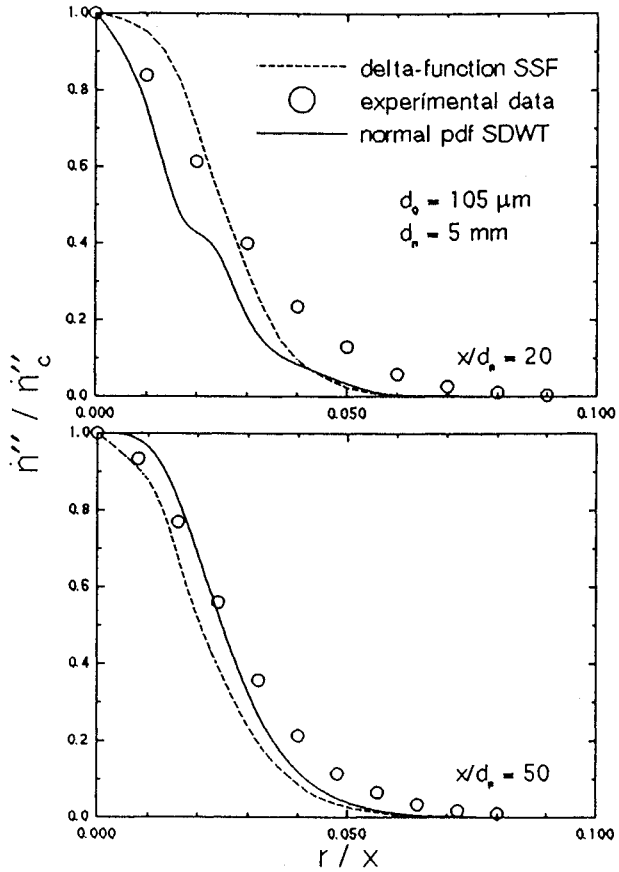

Fig. 3 Time-averaged drop number flux radial profiles ($d_0 = 105$ μm).

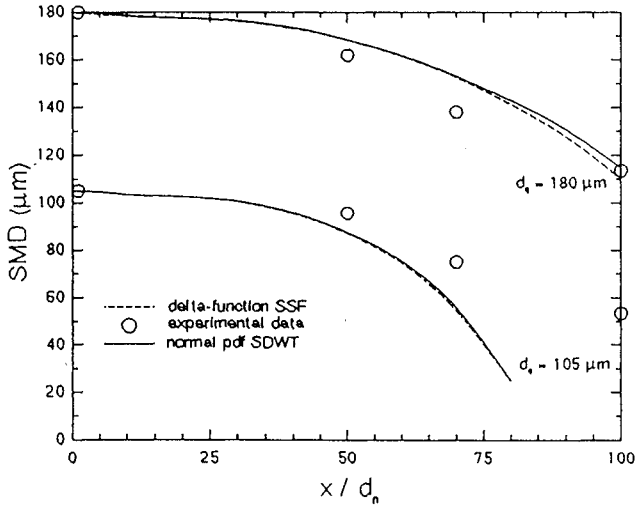

Fig. 4 Time-averaged SMD along the flame axis.

a normal pdf having a mean of zero with a standard deviation of 0.7 mm for the 105 μm drops and a standard deviation of 0.5 mm for the 180 μm drops. This was done to approximate the measured initial drop number flux distribution.

The particular SSF and SDWT modeling parameters selected for evaluation are summarized in Table 2. For the SSF model, the only real consideration is to insure statistically significant sampling. For the SDWT model, however, the ratio of physical particles to computational parcels should be chosen carefully to avoid undersampling while still obtaining the greatest efficiency possible. In this case, the chosen ratio was based on preliminary calculations using various values. The dispersion width correction factor for the SDWT model was taken as unity for all cases.

SSF and SDWT model predictions of the mean drop number flux along the flame axis are shown with experimental data in Fig. 1. Results for both initial drop sizes are presented. The models give comparable predictions that agree favorably with the data. The primary discrepancy between theory and experiment is related to underprediction in the length of the two-phase flow region by both dispersion models for the initially smaller drop size. This behavior should not be attributed to our neglect of fluctuating scalar properties since similar results were encountered in the SSF analysis of Shuen et al.[4,5] where fluctuating scalar properties were taken into account.

An interesting feature that both models were able to resolve is the higher drop number flux along the spray axis for the smaller initial drop size. This result is related to the initially wider number flux distribution for the smaller drops allowing those injected off-axis to diffuse to the centerline. In contrast, the initially larger drops are more concentrated near the axis at injection and therefore have a greater tendency to diffuse away from the centerline. The SDWT model proves capable of resolving this phenomenon despite the small parcel sample size.

Model predictions for the drop number flux radial profiles are given in Fig. 2 for $d_0 = 180$ μm and in Fig. 3 for $d_0 = 105$ μm. Both models exhibit similar behavior, indicating a tendency to underestimate dispersion as distance from injection increases. In fact, the smaller drops were predicted to vaporize completely before reaching $x/d_n = 100$ in contradiction with experimental observation. This underestimation in the length and width of the two-phase region is discussed by Shuen et al.[4,5] and is attributed to an overestimation of gasification rates rather than an underprediction in dispersion. In consideration of this deficiency, both dispersion models perform well.

Theoretical results for the mean SMD along the burner axis are illustrated in Fig. 4 with experimental data. Because the

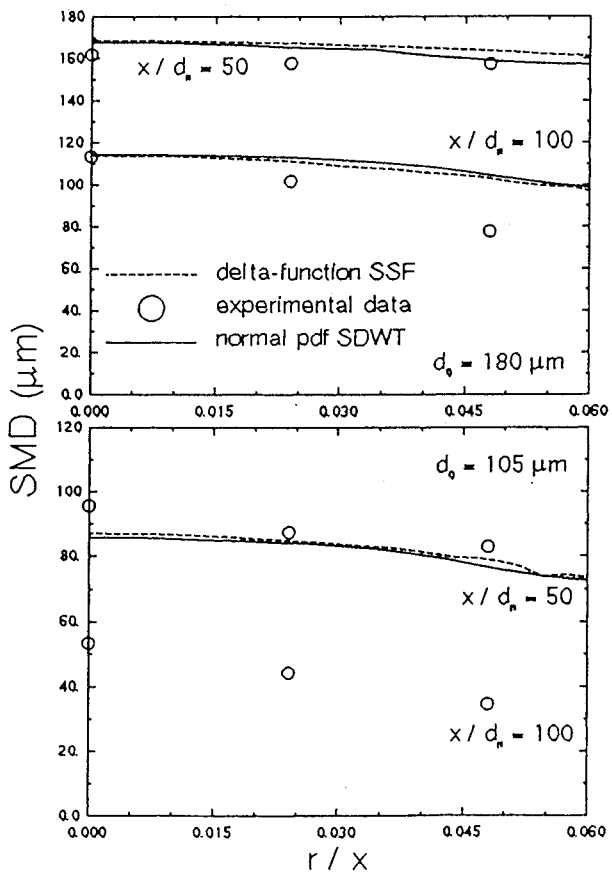

Fig. 5 Time-averaged SMD radial profiles.

spray is monodispersed, the SMD continually decreases with distance from the burner. Predictions from both dispersion models are almost identical. Agreement is good for the initially larger drop size. For the initially smaller drop size, however, the length of the two-phase flow region is greatly underestimated as previously noted.

Predictions for the SMD radial profiles at $x/d_n = 50$ and 100 are given in Fig. 5. Again, both theoretical models provide very similar results. Discrepancies with experimental data are presumably associated with the predicted vaporization rates. This difficulty appears equally troubling to both models—especially near the high gradient flame region.

Conclusion

Based on our evaluation, the proposed SDWT turbulent spray model may be easily extended to dilute combusting sprays with satisfactory results. Global spray structure predictions are as good as for the SSF method with significant improvement in computational efficiency. Model agreement with experimental measurements was good in most cases. Discrepancies between theory and experiment involve underestimation of the length and width of the two-phase flow region and overestimation of drop transport rates near the flame zone for small drops. These difficulties are attributed to the discrete droplet vaporization model rather than the dispersion model. They should not be associated with a neglect of fluctuating scalar properties since results from a previous study[4,5] accounting for such fluctuations yielded similar behavior.

Although the basic results of the evaluation are favorable with regard to the SDWT method, there are special considerations that should be addressed in using the technique. For instance, the possibility of the pdf widths becoming too large in high gradient regions may pose problems in certain cases. There is also the question of treating flows with recirculation. It seems intuitively reasonable to apply the SDWT model as long as the characteristic pdf width is much smaller than the characteristic width of the recirculation region, but a definitive criterion is lacking. From the promising results obtained thus far, however, it does appear that the technique can eventually be developed to make practical spray combustion computations at reduced computational costs.

Acknowledgments

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References

[1]Litchford, R. J., and Jeng, S.-M., "Efficient Statistical Transport Model for Turbulent Particle Dispersion in Sprays," *AIAA Journal,* Vol. 29, No. 9, 1991, pp. 1443–1451.

[2]Litchford, R. J., and Jeng, S.-M., "Efficiency of a Statistical Transport Model for Turbulent Particle Dispersion," *AIAA Journal,* Vol. 30, No. 5, 1992, pp. 1434–1438.

[3]Litchford, R. J., and Jeng, S.-M., "Probability Density Function Shape Sensitivity in the Statistical Modeling of Turbulent Particle Dispersion," *AIAA Journal,* Vol. 30, No. 10, 1992, pp. 2546–2549.

[4]Shuen, J.-S., Solomon, A. S. P., and Faeth, G. M., "Drop-Turbulence Interactions in a Diffusion Flame," *AIAA Journal,* Vol. 24, No. 1, 1986, pp. 101–108.

[5]Shuen, J.-S., Solomon, A. S. P., and Faeth, G. M., "The Structure of Dilute Combusting Sprays," NASA CR-174838, Jan. 1985.

[6]Jeng, S.-M., and Faeth, G. M., "Species Concentrations and Turbulence Properties in Buoyant Methane Diffusion Flames," *Journal of Heat Transfer,* Vol. 106, Nov. 1984, pp. 721–727.

[7]Bilger, R. W., "Turbulent Jet Diffusion Flames," *Progress in Energy and Combustion Science,* Vol. 1, Pergamon Press, New York, 1976, pp. 87–109.

[8]Lockwood, F. C., and Naguib, A. S., "The Prediction of the Fluctuations in the Properties of Free, Round-Jet, Turbulent, Diffusion Flames," *Combustion and Flame,* Vol. 24, No. 1, 1975, pp. 109–124.

[9]Bilger, R. W., "Reaction Rates in Diffusion Flames," *Combustion and Flame,* Vol. 30, No. 3, 1977, pp. 277–284.

[10]Liew, S. K., Bray, K. N. C., and Moss, J. B., "A Flamelet Model of Turbulent Non-Premixed Combustion," *Combustion Science and Technology,* Vol. 27, Dec. 1981, pp. 69–73.

Interaction Between Chemical Reaction and Turbulence in Supersonic Nonpremixed H_2-Air Combustion

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Introduction

In the last decade a number of numerical schemes capable of solving the complete two-dimensional Navier-Stokes equations coupled with chemical reaction have been developed for both confined and unconfined compressible flows. These efforts have focused more on improving numerical efficiency than on developing new physical models for turbulent combustion. Recent studies[1,2] have shown that the lower-upper successive overrelaxation scheme (LU-SSOR) is computationally efficient for reacting supersonic flows.

In many applications of the aforementioned codes to supersonic turbulent combustion, the mean chemical reaction rates are evaluated simply based on Arrhenius expressions with the mean values of temperature and species concentration. Therefore, the potential impact of turbulent fluctuations in temperature and species on chemical reactions has not been considered, and we will refer to such an approach as the *laminar chemistry* model. It has been well known that, in subsonic turbulent combustion, the neglect of the fluctuation effects on the mean chemical reaction rates can lead to erroneous predictions of chemical processes, giving incorrect ignition point or species concentrations. However, modeling the effects of turbulence on chemical kinetics remains unresolved, and it is still an area of intense research efforts.[3] To evaluate the potential impact of turbulence on various chemical processes in supersonic turbulent reacting flows, an approximation is developed to account for the influence of temperature and species fluctuations in the limit of weak turbulence. This approach seems especially appropriate for supersonic nonpremixed turbulent flames where the turbulent mixing is less vigorous than its counterpart in subsonic flows; however, the method only permits qualitative features to be studied. With this approximation, we will concentrate this study on the level of radial concentrations and the point of ignition in supersonic turbulent nonpremixed hydrogen jet flames.

Influence of Turbulence on Chemical Reaction

The effect of small fluctuations in temperature and species concentration can be incorporated into numerical predictions by modifying the Arrhenius chemical source terms as

$$\tilde{w}_A = -\rho^2 M_A \tilde{K}_f \frac{\tilde{Y}_A \tilde{Y}_B}{M_A M_B} (1 - \alpha_{AB})$$

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