Evaluation of NO_x Prediction-Correlation Equations for Small Gas Turbines

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There is strong pressure on both industry and government regulating agencies to reduce, control, and predict pollutants from gas turbine engines. Several available prediction-correlation methods for NO_x were examined and tested with small gas turbine data. In addition, an alternate approach was used to develop a new NO_x equation. No one equation could be found that was satisfactory for even a small group of engines, much less for all engines. It was possible, however, to find at least one NO_x correlation equation for any specific engine that will predict NO_x within 5-20% over the full range of engine operation. The significance of the study is that a more precise prediction method than a single equation will probably be required in order to adequately predict NO_x over an entire engine cycle from one laboratory test condition. However, for small corrections which are used to transpose engine data to standard-day conditions, most of the equations studied are probably adequate.

Nomenclature

A	= combustor flow area
f	= fuel-air ratio
H	= humidity in lb H ₂ O/lb air
K	= correlation equation adjustment coefficient
K_f	= reaction rate coefficient, defined by Eq. (4)
[ŃO]	= brackets indicate concentration of gaseous component in mols/cc
(NO)	= parantheses indicate volumetric fraction of
, ,	gaseous component
P	= pressure in absolute units
R_{θ}	= universal gas constant
T_B	= burner or combustor average exit temperature
T_B T_S	= peak adiabatic flame temperature (°R or K) for stoichiometric mixture, calculated
$T_{\mathfrak{Z}}$	= combustor inlet air temperature in absolute units, °R
V	= velocity
W_a	= air mass flow rate
α	= function of Zeldovich reaction $N + 0_2 = NO + O$ (Eq. 2)
γ	= defined by Eq. (2)
ϕ	= equivalent ratio = $f/f_{\text{stoichiometric}}$
au	= chemical reaction time for NO
Subscript	

Introduction and Background

= reference point

BOTH government and the gas turbine industry are concerned with the measurement of gas turbine emissions, the setting of achievable low emission levels, and standardization of methods for determining when compliance has been met. This paper is a result of a study to apply existing and new equations for the prediction and correlation of NO_x . Data from small Avco Lycoming gas turbine engine combustors were used to evaluate the equations. Our objective

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was either 1) to find a universal NO_x correlation equation, or 2) to demonstrate the accuracy of such existing prediction methods.

Attempts by several investigators to develop NO_x prediction and correlation equations have been successful, at least in part, for some gas turbine engines. Lipfert plotted NO_x data from many aircraft gas turbine engines versus compressor air discharge temperature (T_3) and produced a good correlation. However, small Lycoming engines have different slopes and trends (Fig. 1). The difference between these Lycoming data and the general trend for the group of gas turbine data that were plotted from Lipfert is sufficient to cause large errors in extrapolating and predicting NO_x emissions from Lycoming engines. This is particularly true when Federal EPA compliance error tolerance is small. In addition, single-shaft constant-speed engines operate at nearly constant compressor discharge temperature (T_3) , and therefore have an entirely different NO_x correlation.

Several investigators have examined more detailed NO_x prediction and correlation approaches. A summary of NO_x prediction-correlation methods is given by Sullivan, ² and is followed by an equation proposed by Sullivan. ³ Other NO_x prediction equations have been proposed by Marchionna et al. ⁴ Davis et al., ⁵ Vermes, ⁶ Sarli et al., ⁷ Cohen, ⁸ Kretschmer and Odgers, ⁹ Touchston and Dibelius, ^{10,11} and others. Shaw's analysis of the kinetics of NO (or NO_x) formation ¹²

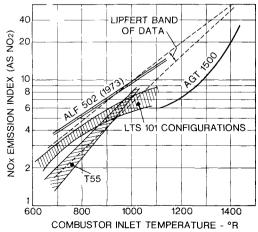


Fig. 1 NO_x emission index of Avco Lycoming small gas turbines vs Lipfert group of data, humidity = 0.

has been widely used by many investigators. These investigators proposed equations which evaluated several of the known combustor NO_x producing factors, and compared or adjusted these factors to experimental data. A tabulation of the factors in these equations is shown in Table 1. Others have developed more complex modeling methods for NO_x prediction. One of these, of moderate complexity, was developed by Hung, 13,14 and shown to be applicable to the limited group of engines which he used to test the method.

Table 1 shows that pressure, air and gas temperature, residence time, and air mass flow parametric effects differ as evaluated by individual investigations. One may conclude that selecting correlating parameters is not a simple matter. The reason that precise prediction of NO_x is complex can be appreciated by examining the processes in the combustor regions (Fig.2). The primary zone is conceded to be the hottest region of the combustor and the principal place where NO is formed.

In the present investigation, we examine some of the more promising NO_x prediction-correlation equations, develop an alternate equation, and evaluate these equations for use with Avco Lycoming small gas turbines. Five equations were selected as typical of those available. Three different types of Lycoming combustors were used in the analysis. With one engine, three fuels were evaluated.

Development of an Alternate NO_x Equation

In the process of NO_x equation evaluation, the authors investigated a somewhat different NO_x prediction approach based on physical chemistry with simplifying assumptions. The assumptions for this model are reduced to:

1) The controlling NO formation reaction is the Zeldovich reaction:

$$O + N_2 \rightleftharpoons NO + N \tag{1}$$

Marteney ¹⁵ made the additional simplifying assumptions that the NO and N concentrations are zero intially, and arrived at the equation

[NO]_{$$\tau$$} = $2\gamma\tau - (\gamma/\alpha)(I - e^{-\alpha\tau})$ (2)

where γ is a function of the Zeldovich reaction [Eq. (1)] and α for the Zeldovich reaction $(N+O_2 \rightleftharpoons NO+O)$. He shows that Eq. (1) is dominant for conditions typically found in gas turbine combustors, and that for longer combustor residence times where $\alpha\tau > 3$, Eq. (2) reduces to:

$$[NO]_{\tau} \cong 2\gamma\tau \tag{3}$$

where $\gamma = K_f[N_2][O]$ and K_f is the rate coefficient (Ref. 15):

$$K_f = (7.0 \times 10^{13}) \exp(-38,000/T_s)$$
 (4)

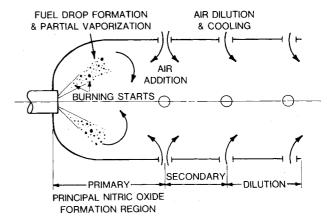


Fig. 2 Combustor schematic showing nitric oxide formation zone.

- 2) The oxygen radical concentration rises rapidly and reaches a partial equilibrium state, while the NO rises slowly. The O-radical can thus be considered to be at temporary equilibrium, and its concentration can be determined from equilibrium tables for conditions present in the combustor primary zone.
- 3) Pressure affects the kinetics as calculated by Marteney (Ref. 15), where

$$(NO)_{\text{equil}} \propto P^{-0.21} \tag{5}$$

- 4) The peak NO formation rate occurs at stoichiometric fuel-air ratio ($\phi = 1$). ¹⁶ The NO rate drop-off either side of stoichiometric is rapid. We can assume that all of the NO is formed in the stoichiometric mixture burning regions, as proposed by Kretschmer and Odgers. ⁹
- 5) Combustor residence time, effective in producing NO, is based on the assumption that the NO formed in the primary zone at peak gas temperature is suddenly quenched, or its rate drastically reduced, at the first large airjet mixing station of the combustor. The gas residence time at NO-producing temperature is thus.

$$\tau \propto 1/V \propto P/T W_a \tag{6}$$

where T is the combustion gas temperature.

The combustor overall fuel-air ratio is introduced as a dilution factor only. From the assumption that all of the NO is formed at $\phi=1$, the reacting gases are cooled and diluted to the reduced overall combustor exit fuel-air ratio as they progress through the combustor, so that:

$$(NO)_{exhaust} \propto f(combustor average)$$
 (7)

In the process of developing the final equation, the fuel-air dilution effect cancels the fuel-air ratio effect determined from the NO residence time.

Table 1 Comparison of equation factors affecting NO, production

Reference	Pressure	Temperature	Time	Fuel-Air	Mass	Other
Shaw	$P^{0.5}$	$\exp(1/T_R)$	τ			(NO) _{eq.}
Marchionna et al.	$P^{1.5}$	$T_3^{5} \exp T_3$		f	W_{σ}^{-1}	· · · · · · · · · · · · · · · · · · ·
Davis et al.	$P^{0.29}$	$\exp T_3$		$f^{1.48}$	$W_{a}^{-0.1}$	
Vermes	$P^{1.5}$	$\exp \Delta T_3$	$ au^{\mathrm{a}}$	$f-f_0$	W_{a}^{-1}	
Sarli et al.	$P^{0.5}$	$\exp T_3$		f	ű	
Cohen	P	$T_{3}^{6.25}$		$(I+f)^{-1}$	W_{α}^{-1}	
Lipfert (approx.)	$P^{0.5}$	$\exp T_3$		f	ű	
Kretschmer, Odgers		$T_3, \Delta T_{\phi=1}$		•		
Touchston, Dibelius	$P^{0.5}$	$\exp(\Delta T_3 + I/\Delta T_3)$	au	f , $\exp(\Delta f)$		
Sullivan	$P^{0.5}$	$\exp \Delta T_3$		$f^{1.4}$	$W_a^{-0.22}$	
Present work	$P^{0.79}$	$\exp(-1/T_S), T_S^{-1}$	au	$f/f_{\rm stoich.}$. **	(O) _{eq.}

^a $\tau \sim P/W_a$, $f_0 = \text{fuel/air at (NO}_x = 0)$.

6) Air humidity effect has been empirically evaluated and was obtained from Ref. 4:

$$(NO)_1/(NO)_2 = \exp[19(H_2 - H_1)]$$
 (8)

7) The dominant nitrogen gas produced from kinetic rate equations is NO. Some NO_2 formation can be predicted, but is usually a small amount. We assume that the total NO_x product $(NO + NO_2)$ is proportional to the NO formed, so that:

$$(NO_x)_1/(NO_x)_2 = (NO)_1/(NO)_2$$
 (9)

By combining these effects and converting mols/cc to volume fraction via the gas law, where

$$[N_2] = P(N_2)/R_0T_s$$
$$[O] = P(O)/R_0T_s$$

where $P(N_2)$ and P(O) are partial pressure of N_2 and Oradical respectively, we obtain

$$(NO_x)/(NO_x)_R = \{ \exp[3.8 \times 10^4 (1/T_{sR} - 1/T_s)] \}$$

$$\times [(P/P_R)^{1.79} ((O)/(O)_R)$$

$$\times (W_{aR}/W_a) (T_{sR}/T_s)] \exp[19(H_R - H)]$$
(10)

The peak gas stoichiometric temperature, T_s , is also calculated from Refs. 17 or 18 and is used to select values of O.

Other Equations Used in the Evaluations

The additional equations selected for further examination were regarded as typical, based on theory or on reasonable empiricism. The reader should refer to the individual papers for a detailed discussion of equation development. Our purpose was to evaluate the precision of the selected group as applied to Lycoming's small gas turbine combustors.

Sarli, Eiler, and Marshall Equation 7

This equation was also developed using the Zeldovich NO formation reaction [Eq. (1)] as suggested by Marteney. Residence time was not regarded as an important factor, and the resultant equation, including water vapor effect, is

$$(NO_x)/(NO_x)_R = (P/P_R)^{0.5} \exp[0.00313(T-T_R)]$$

$$\times \exp[19(H_R - H)][(1 + 1/f_R)/(1 + 1/f)] = A$$
 (11)

Variations on the Sarli equation included adding a combustor residence time factor, τ , where

$$\tau/\tau_R = \sqrt{T_{BR}/T_B} \tag{12}$$

and

$$(NO)_x/(NO_x)_R = A\sqrt{T_{BR}/T_B}$$
 (13)

The time-variation factor suggested by Touchton and Dibelius [Eq. (17)] was also tried, where

$$(NO_x)/(NO_x)_R = A(P/P_R)(f_R/f)(W_{aR}/W_a)$$
 (14)

Sullivan Equation³

Sullivan's equation is based on experimental evaluation of the exponents of pressure, fuel-air ratio, and mass flow:

$$NO_x/NO_{xR} = (P/P_R)^{0.5} (f/f_R)^{1.4} (W_{aR}/W_a)^{0.22}$$

 $\times \exp([T-T_R]/396) \exp[19(H_R-H)]$ (15)

where T is inlet air temperature in °R. From Ref. 3, we note that this equation predicts NO_x well for some large constant speed industrial gas turbine engines, and not so well for others, such as the variable speed JT-9D.

Touchston and Dibelius 10.11

The model assumptions proposed by Shaw¹² were used to develop an equation based on chemical kinetics (plug flow) and a constant residence time, using the Zeldovich reactions for NO formation. Curve-fitting constants were used to write the final equation in terms of $P_{s}f_{s}T_{s}$, and H:

$$NO_x/NO_{xR} = (f/f_R) (P/P_R)^{0.5} \exp([T_3 - T_{3R}]/380)$$

 $\times \exp[39,300(f/T_3 - f_R/T_{3R})] \exp[19(H_R - H)]$ (16)

A modification of this equation is obtained by including combustor residence time as a function of combustor mass flow:

$$(NO_x)/(NO_x)_R = (W_{aR}/W_a) (P/P_R)^{1.5} \exp([T-T_R]/380)$$

$$\times \exp[39,000(f/T-[f/T]_R)] \exp[19(H_R-H)]$$
 (17)

The factor 39,000 is considered a "configuration" factor, and was so used in Ref. 11. By modifying this factor D, configuration effects can be included.

Marchionna et al.4

This equation was based on experimental data taken at constant combustor inlet Mach number, constant exhaust gas temperature, and variable inlet temperature, using a 40 in. diameter Pratt and Whitney research combustor. A limited amount of experimental data was taken to verify the assumed variation of NO_x with pressure to the 0.5 power and inlet Mach number to the -1 power.

$$(NO_x)/(NO_x)_R = \exp[I.14([T_3 - T_{3R}]/520)] \times W_{aR}/W_a) (P/P_R)^{1.5} (T_{3R}/T_3) 0.5 \times (f/f_R) ([I+f_R]/[I+f]) \exp[I9(H_R - H)]$$
(18)

where T_3 is in °R.

Configuration Adjustment Factor

From our analysis thus far, it becomes obvious that none of the equations examined will predict a priori the NO_x concentration for the full range of engine combustor operation. By calculating the ratio NO_x/NO_{xR} , in which NO_{xR} is an

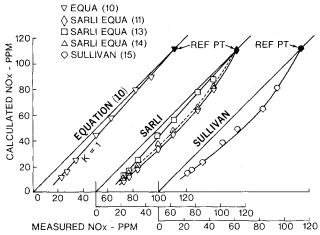


Fig. 3 LTP 101 correlation of measured vs calculated ${\rm NO}_x$ (JP-5 fuel, humidity = 0).

experimentally determined point, we can determine the NO_x at other conditions, providing that the extrapolation is within an established error limit. An extrapolation using a NO_R point is shown in Fig. 3. If NO_R is selected at the high-power end of operation, extrapolation to the low-power end produces some error. However, we can see that if the extrapolation is short, a small correction factor can be added to the equation that will produce very close correlation of NO_x values. The difference between measured results and calculated results can be attributed to a "configuration" factor. This is handled by the Touchston-Dibelius equation with a variable D factor. The method chosen by the present authors was to select *two* NO_{xR} values at opposite ends of the power spectrum, and to examine the data for deviation from linear interpolations.

The NO_x values can then be calculated from the equation

$$(NO_x)_{corr.} = [(NO_x)_R/K][K-I+(NO_x)/(NO_x)_R]$$
 (19)

where K is a slope term determined from two measured and two calculated values of NO_x .

Experimental Data

The NO (or NO_x) correlation-prediction equations were applied to data from three Avco Lycoming engines with combustors of different design, and for different engine cycle operating conditions. These engines are all two-shaft, free-power turbine designs. The combustor configurations were from these engines.

- 1) The LTP 101 is a small gas turbine in the 600 shp range, using an annular combustor with several large turbulence-generating wall jets, producing a unique aerodynamic pattern.
- 2) The ALF 502 is a high-bypass-ratio turbofan engine, with the combustor operating at inlet pressures up to 12 atm. The combustor is also annular, but more conventional in design.
- 3) The AGT 1500 engine is a 14.5:1 pressure ratio recuperative engine with combustor inlet temperature over 1000°F. The combustor is can-type.

Data were obtained for both engine and combustor laboratory tests. NO_x data were taken with sampling systems using a chemiluminescence detector for NO and NO_x , following the procedures recommended by the EPA in CFR 40, Part 87.

Discussion of Results

The equations were evaluated by comparing measured NO_x with calculated NO_x from one of the correlation equations. In some cases, a reference value was selected at a high NO_x value. In others, a reference at high NO_x and a second reference at a low NO_x value were selected and the coefficient K was used in making this adjustment. "Good" correlation was defined by 1) a 5-10% deviation from the 1:1 correlation line with a single point reference, or 2) 5-10% of nonlinearity when two reference points were used.

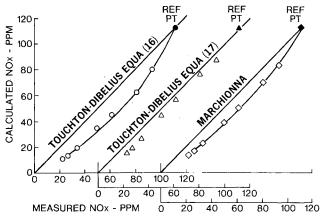


Fig. 4 LTP 101 correlation of measured vs calculated NO_x (JP-5 fuel, humidity = 0).

LTP 101 Results

The plotted correlations for this engine are shown in Figs. 3 and 4 for the five equations evaluated. Of these, Eq. (10) produces precision within 5% after the correction factor was applied. The Sarli et al equation (13), with a residence time modification, also produced a straight-line correlation. With application of the K factor, 5% accuracy could be reached.

Several of the equations, including the Sullivan equation (15), produce correlations that deviate by a nonlinear function. A correction factor addition in this situation is not simple. The Touchston-Dibelius correlation, Eq. (16), produces poor correlation, but after introducing the time function, correlation was improved. Still further improvements were realized by changing the *D* configuration factor

The results are summarized in Table 2. We conclude that Eqs. (10), (14), and (17) all produce correlations for the LTS 101 with potential accuracy over the full engine operating range of 5%.

ALF 502 Results

The correlations for this engine are summarized in Table 3. As shown, relatively poor correlations are produced by *all* of the equations. The most promising is the Marchionna equation, which can be fitted to the data by using the linear correction, Eq. (19), with an accuracy potential of 5%. Application of the Marchionna equation to the ALF 502 is shown in Figs. 5 and 6, both with and without the linear correction applied

AGT 1500 Results

This engine was tested with JP-4, JP-5, and DF-2 fuel. The NO_x data are similar for all three fuels. This is not surprising, considering the high combustor inlet air temperature from the recuperator.

Table 2 LTP 101 NO_x correlation equation evaluation

	•	Full operating range prediction accuracy		
Equation	Time factor, τ	No correction factor	With correction factor	
Present work (10)	Function of mass flow	40%	5%	
Sarli et al. (11)	None	50%		
Sarli et al. (13)	Function of mass flow	40%		
Sarli et al. (14)	Function of $\sqrt{I/T_d}$	40 %	5 %	
Sullivan (15)	None	35%		
Touchston-Dibelius (16)	Function of mass flow	45 %		
Touchston-Dibelius (17)	Do	30%(D constant)	5 %	
Touchston-Dibelius (17)	Do	30%(D variable)		
Marchionna et al. (18)	Function of M^{-1}	40%		

Table 3 ALF 502 NO_x correlation equation evaluation

	Full operating range prediction accuracy		
Equation	No corr. factor	With corr.	
Present work (10)	± 20%		
Sarli et al. (11)	50%		
Sarli et al. (13)	30%		
Sarli et al. (14)	$\pm 20\%$		
Sullivan (15)	30%		
Touchston-Dibelius (16)	45%		
Touchston-Dibelius (17)	+15% -20%		
Touchston-Dibelius (17)	+7% -20%		
. ,	D = 30,000		
	and 40,000		
Marchionna et al. (18)	-25%	5 %	

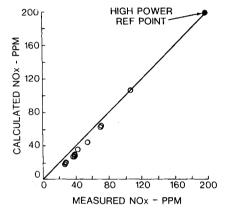


Fig. 5 ALF 502 engine NO_x , Marchionna equation without slope correction factor (JP-5 fuel, humidity = 0).

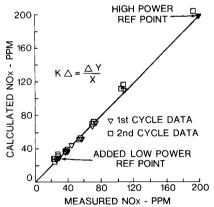
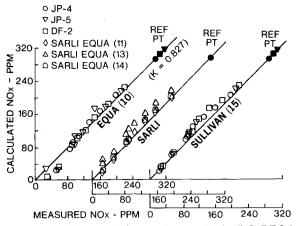


Fig. 6 ALF 502 engine NO_x , Marchionna equation with slope correction factor (K) applied (JP-5 fuel, humidity = 0).

From Figs. 7 and 8 and the summary in Table 4, we find that the best correlation is obtained from the Sarli et al. equation without a combustor residence time correction, which is contradictory with the precision of this equation applied to the LTP 101. Other reasonable correlations are obtained with the Touchston-Dibelius equation without the residence time factor. Improvement with the Touchston-Dibelius equation could be obtained by changing the configuration coefficient. Equation 10 (present work) can be adjusted to produce good correlation, only at the high-power end of the plot.

Comparison with Other Engines

Equation 10 was used for correlations by the authors of Ref. 10 with General Electric MS 7001C (simple cycle) and a



AGT 1500 engine NO_x correlations (JP-4, JP-5, DF-2 fuel, humidity = 0).

- o TOUCHTON-DIBELIUS EQUA (16), JP-4 TOUCHTON-DIBELIUS EQUA (17), JP-4 □ MARCHIONNA, JP-4
- ♦ MARCHIONNA, JP-5 ▲ MARCHIONNA, DF-2

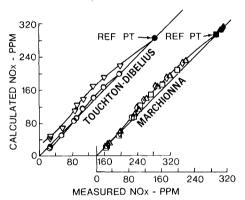


Fig. 8 NO, correlation for AGT 1500 (JP-4, JP-5, DF-2 fuel, humidity = 0).

Table 4 AGT 1500 NO., correlation equation evaluation

Equation	Full operating range prediction accuracy
Present work (10)	+ 15% or more, nonlinear
Sarli et al. (11)	$+5\%_0, -20\%_0$
Sarli et al. (13)	± 10%
Sarli et al. (14)	+ 50%, nonlinear
Sullivan (15)	+ 20%, nonlinear
Touchston-Dibelius (16)	$+7\%_0, -15\%_0$
Touchston-Dibelius (17)	+ 30%
Touchston-Dibelius (17)	$\frac{+}{2}$ 10% with D factor
Marchionna et al. (18)	+ 15%, nonlinear

7001B (regenerative cycle) engine. These are constant-speed industrial-type engines. This correlation indicates that Eq. (10) may have application to large constant-speed engines. Further work is required to establish constant-speed engine use for Eq. 10.

Summary and Conclusions

Many attempts have been made to arrive at and evaluate equations for predicting and correlating gas turbine NO_x data. The authors have evaluated some of these as applied to Avco Lycoming small gas turbine data. A newly developed additional equation has also been evaluated. The accuracy demanded of these equations is high because of 1) demands of regulating agencies for reduced emissions and a "universal" correlation method and 2) the desire of engine manufacturers to be able to make precise predictions of emissions.

The analysis of these equations clearly shows that none of the single-equation prediction-correlations are universally applicable to wide operating range predictions for all combustors and engine cycles. Most of the equations are satisfactory when used for small corrections normally required in adjusting emissions data to standard-day conditions. It also shows that, by cut-and-try, one or more equations can be found that can be applied to a specific engine and combustor and produce "good" correlation capability—to within 5-10% of the measured value.

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RADIATIVE TRANSFER AND THERMAL CONTROL—v. 49

Edited by Allie M. Smith, ARO, Inc., Arnold Air Force Station, Tennessee

This volume is concerned with the mechanisms of heat transfer, a subject that is regarded as classical in the field of engineering. However, as sometimes happens in science and engineering, modern technological challenges arise in the course of events that compel the expansion of even a well-established field far beyond its classical boundaries. This has been the case in the field of heat transfer as problems arose in space flight, in re-entry into Earth's atmosphere, and in entry into such extreme atmospheric environments as that of Venus. Problems of radiative transfer in empty space, conductance and contact resistances among conductors within a spacecraft, gaseous radiation in complex environments, interactions with solar radiation, the physical properties of materials under space conditions, and the novel characteristics of that rather special device, the heat pipe—all of these are the subject of this volume.

The editor has addressed this volume to the large community of heat transfer scientists and engineers who wish to keep abreast of their field as it expands into these new territories.

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