Setting Prompt NO_x Parameters

Prompt NO_x formation is predicted using Equation 13.1-25 and Equation 13.1-27 in the separate Theory Guide. For each fuel stream specified in the Fuel Stream ID text box in the Formation tab, set the parameters in the Prompt tab under Formation Model Parameters in the NOx Model dialog box in the following manner:

- Set the Fuel Carbon Number to specify the number of carbon atoms per fuel molecule.
- Set the Equivalence Ratio as follows:

$$\text{Equivalence Ratio} = \frac{\text{actual fuel-to-air ratio}}{\text{stoichiometric fuel-to-air ratio}}$$

  For any carbon number, C_n, the limits of the Equivalence Ratio are such that, if it is greater than 1.57, then limit the Equivalence Ratio to 1.57. If C_n is less than or equal to 4, then an additional limit is applied. When the Equivalence Ratio is between 0.365 and 0.685, the midpoint value is computed, which is 0.525. Thus for Equivalence Ratio values below the midpoint value, set the value to the lower limit and for an Equivalence Ratio above the midpoint value, set the value to the upper limit). These limits are purely mathematical and only guarantee positive prompt NO_x rates.

If you hooked a UDF in the Formation tab, you can make a selection in the UDF Rate group box to specify the treatment of the user-defined NO_x rate:

- Select Replace FLUENT Rate to replace ANSYS FLUENT's prompt NO_x rate calculations with the custom NO_x rate produced by your UDF.
- Select Add to FLUENT Rate to add the custom NO_x rate produced by your UDF to ANSYS FLUENT's prompt NO_x rate calculations.

Setting Fuel NO_x Parameters

When using the fuel NO_x model, you must set the parameters in the Fuel tab under Formation Model Parameters for each fuel stream specified in the Fuel Stream ID text box in the Formation tab.

If you hooked a UDF in the Formation tab, you can make a selection in the UDF Rate group box to specify the treatment of the user-defined NO_x rate:

- Select Replace FLUENT Rate to replace ANSYS FLUENT's fuel NO_x rate calculations with the custom NO_x rate produced by your UDF.

- Select Add to FLUENT Rate to add the custom NO_x rate produced by your UDF to ANSYS FLUENT's fuel NO_x rate calculations.

If there is no NO_x rate UDF or if you selected Add to FLUENT Rate, you must define fuel parameters. To begin, specify the fuel type in the following manner:

- For solid fuel NO_x, select Solid under Fuel Type.
- For liquid fuel NO_x, select Liquid under Fuel Type.
- For gaseous fuel NO_x, select Gas under Fuel Type.

Note that you can use only one of the fuel types for a given fuel stream. The Gas option is available only when the Species Transport model is enabled (see Section 15.1.2: Enabling Species Transport and Reactions and Choosing the Mixture Material).

Setting Gaseous and Liquid Fuel NO_x Parameters

If you have selected Gas or Liquid as the Fuel Type, you will also need to specify the following:

- Select the intermediate species (hcn, nh3, or hcn/nh3/no) in the N Intermediate drop-down list.
- Set the correct mass fraction of nitrogen in the fuel (kg nitrogen per kg fuel) in the Fuel N Mass Fraction field.
- Specify the overall fraction of the fuel N, by mass, that will be converted to the intermediate species and/or product NO in the Conversion Fraction field. The Conversion Fraction for the N Intermediate has a default value of 1. Thus, any remaining N will not contribute to NO_x formation. This is based on the assumption that the remaining volatile N will convert to gas phase nitrogen. However, this has very little effect on the overall mass fraction of gas phase nitrogen. Therefore, you do not have to solve for nitrogen species when solving pollutant transport equations.
- If you selected hcn/nh3/no as the intermediate, specify the fraction of the converted fuel N, by mass, that will become hcn and nh3 under Partition Fractions. The fraction of fuel N that will become NO will be calculated by the remainder.

  Note that setting a partition fraction of 0 for both HCN and NH_3 is equivalent to assuming that all fuel N is converted to the final product NO, whereas a partition fraction of 0 for HCN and 1 for NH_3 is the same as selecting nh3 as the intermediate.

ANSYS FLUENT will use Equation 13.1-29 and Equation 13.1-30 (in the separate Theory Guide) (for HCN) or Equation 13.1-40 and Equation 13.1-41 (in the separate Theory Guide) (for NH_3) to predict NO formation for a gaseous or liquid fuel.

Note that there is a limitation that must be considered when defining more than one liquid fuel stream. See Section 21.1.1: Defining the Fuel Streams for details.

Setting Solid (Coal) Fuel NO_x Parameters

For solid (coal) fuel, ANSYS FLUENT will use Equation 13.1-54 and Equation 13.1-55 (in the separate Theory Guide) (for HCN) or Equation 13.1-61 and Equation 13.1-62 (in the separate Theory Guide) (for NH_3) to predict NO formation. Several inputs are required for the coal fuel NO_x model as follows:

- Select the intermediate species (hcn, nh3, or hcn/nh3/no) in the N Intermediate drop-down list.
- Specify the mass fraction of nitrogen in the volatiles in the Volatile N Mass Fraction field.
- Specify the overall fraction of the volatile N, by mass, that will be converted to the intermediate species and/or product NO in the Conversion Fraction field.
- If you selected hcn/nh3/no as the volatile N intermediate, specify the fraction of the converted volatile N, by mass, that will become hcn and nh3 under Partition Fractions. The fraction of volatile N that will become NO will be calculated by the remainder.
- Select the char N conversion path from the Char N Conversion drop-down list as no, hcn, nh3, or hcn/nh3/no. Note that hcn or nh3 can be selected only if the same species has been selected as the intermediate species in the N Intermediate drop-down list.
- Specify the mass fraction of nitrogen in the char in the Char N Mass Fraction field.
- Specify the overall fraction of the char N, by mass, that will be converted to the intermediate species and/or product NO in the Conversion Fraction field.
- If you selected hcn/nh3/no as the char N conversion, specify the fraction of the converted char N, by mass, that will become hcn and nh3 under Partition Fractions. The fraction of char N that will become NO will be calculated by the remainder.
- Define the BET internal pore surface area (see Section 13.1.5: BET Surface Area in the separate Theory Guide for details) of the particles in the BET Surface Area field.

Note that there are limitations that must be considered when defining more than one solid fuel stream. See Section 21.1.1: Defining the Fuel Streams for details.

The following equations are used to determine the mass fraction of nitrogen in the volatiles and char:

$$\dot{m}_{N_{v/c}} = \dot{m}_{v/c} * mf_{N_{v/c}} \tag{21.1-1}$$

where

$\dot{m}_{N_{v/c}}$ = rate of release of fuel nitrogen in kg/s
$\dot{m}_{v/c}$ = rate of release of volatiles (v) or char (c) in kg/s
$mf_{N_{v/c}}$ = mass fraction of nitrogen in volatiles or char

Let

TN_{fuel} = total nitrogen mass fraction in daf coal (i.e., from daf ultimate analysis)
N_{split} = char nitrogen as a fraction of total nitrogen
F_{vol} = mass fraction of volatiles in daf coal
F_{char} = mass fraction of char in daf coal

Then the following should hold:

$$F_{vol} + F_{char} = 1 \tag{21.1-2}$$

$$\frac{F_{char} * mf_{N_c}}{TN_{fuel}} = N_{split} \tag{21.1-3}$$

$$F_{vol} * mf_{N_v} + F_{char} * mf_{N_c} = TN_{fuel} \tag{21.1-4}$$

$$mf_{N_v} = (1 - N_{split}) * \frac{TN_{fuel}}{F_{vol}} \tag{21.1-5}$$

$$mf_{N_c} = N_{split} * \frac{TN_{fuel}}{F_{char}} \tag{21.1-6}$$

Note that if water is assumed to release at the same rate as volatiles, the above calculation has to be slightly modified.

Setting N_2O Pathway Parameters

The formation of NO through an N_2O intermediate can be predicted by two methods. You will specify the method to be used in the N2O Path tab.

- To choose the quasi-steady state method, select quasi-steady in the N2O Model drop-down list.

  i The transport equation for the species N_2O will not be solved for N_2O, however, N_2O will be updated at every iteration. Therefore, the residual values that appear for N_2O are always zero. Do not be alarmed if the solver keeps printing zero at each iteration.

- To choose the simplified form of the N_2O-intermediate mechanism, select transported-simple in the N2O Model drop-down list. Here, the species N_2O is added to the list of pollutant species, and its mass fraction is solved via a transport equation.

The atomic O concentration will be calculated according to the thermal NO_x [O] Model that you have specified previously. If you have not selected the Thermal NOx pathway, then you will be given the option to specify an [O] Model for the N_2O pathway calculation. The same three options for the thermal NO_x [O] Model will be the available options.

If you hooked a UDF in the Formation tab, you can make a selection in the UDF Rate group box to specify the treatment of the user-defined NO_x rate:

- Select Replace FLUENT Rate to replace the NO_x rate calculated by ANSYS FLUENT using N_2O intermediates with the custom NO_x rate produced by your UDF.
- Select Add to FLUENT Rate to add the custom NO_x rate produced by your UDF to the NO_x rate calculated by ANSYS FLUENT using N_2O intermediates.

Setting Parameters for NO_x Reburn

To enable NO_x reduction by reburning, click the Reduction tab in the NOx Model dialog box and enable the Reburn option under Methods. In the expanded portion of the dialog box, as shown in Figure 21.1.3, click the Reburn tab under Reduction Method Parameters, where you can choose from the following options:

- To choose the instantaneous method, select instantaneous [CH] in the Reburn Model drop-down list.

  i When you use this method, you must be sure to include the species CH, CH_2, and CH_3 in your problem definition. See Section 13.1.7: NOx Reduction by Reburning in the separate Theory Guide for details.

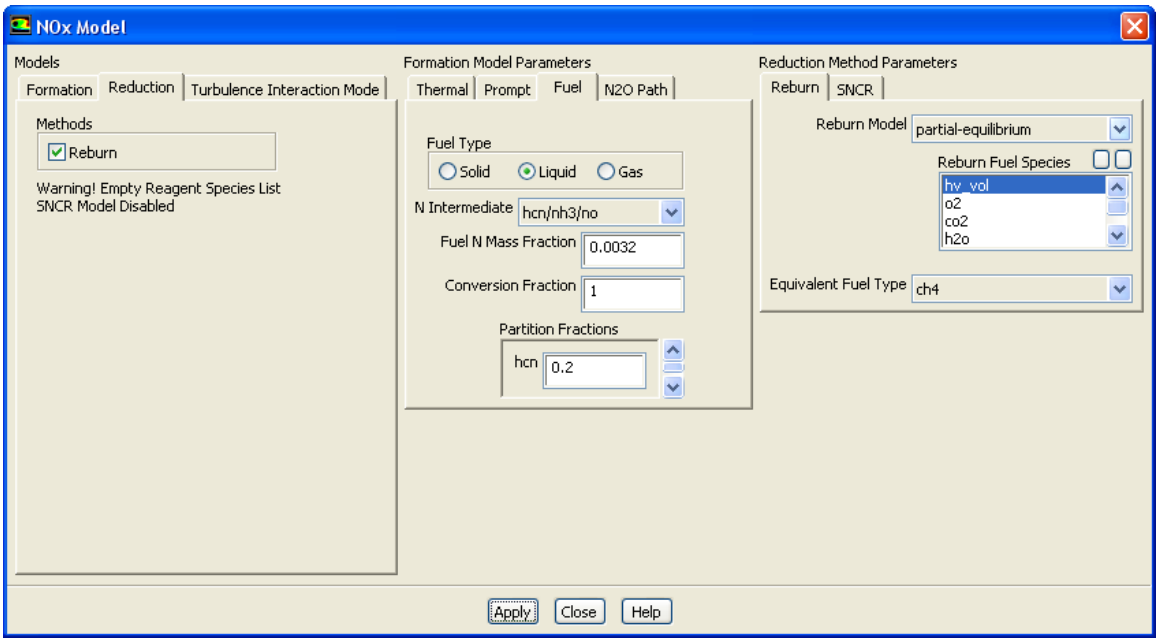

Figure 21.1.3: The NO_x Dialog Box Displaying the Reburn Reduction Method

- To choose the partial equilibrium method, select partial-equilibrium in the Reburn Model drop-down list. You will then need to select the Reburn Fuel Species from the list of available species. ANSYS FLUENT will allow you select up to 5 reburn fuel species. Specify the Equivalent Fuel Type (ch4, ch3, ch2, or ch). For example, if you choose methane as the reburn fuel, then the Equivalent Fuel Type would be ch4. If you choose a reburn fuel such as hv_vol (a volatile component of coal), then you must specify the most appropriate equivalent hydrocarbon fuel type so that the partial equilibrium model will be activated correctly.

- Due to coal volatiles behaving very differently, it is important to select the correct equivalent fuel type. You must first consider the volatile fuel composition, then check the C/H ratio to find the fuel which most closely matches CH, CH_2, CH_3, or CH_4 [43]. How the equivalent fuel is determined is still debatable, however, considering the C/H ratio of the fuel itself is a reasonable indicator.

Setting SNCR Parameters

Prior to enabling reduction by SNCR, make sure that you have included in the species list nh3 (for reduction by ammonia injection) and co<nh2>2 (for reduction by urea injection). See Section 13.1.8: NOx Reduction by SNCR in the separate Theory Guide for detailed information about SNCR theory.

To enable NO_x reduction by SNCR, click the Reduction tab in the NOx Model dialog box and enable the SNCR option under Methods, as shown in Figure 21.1.4.

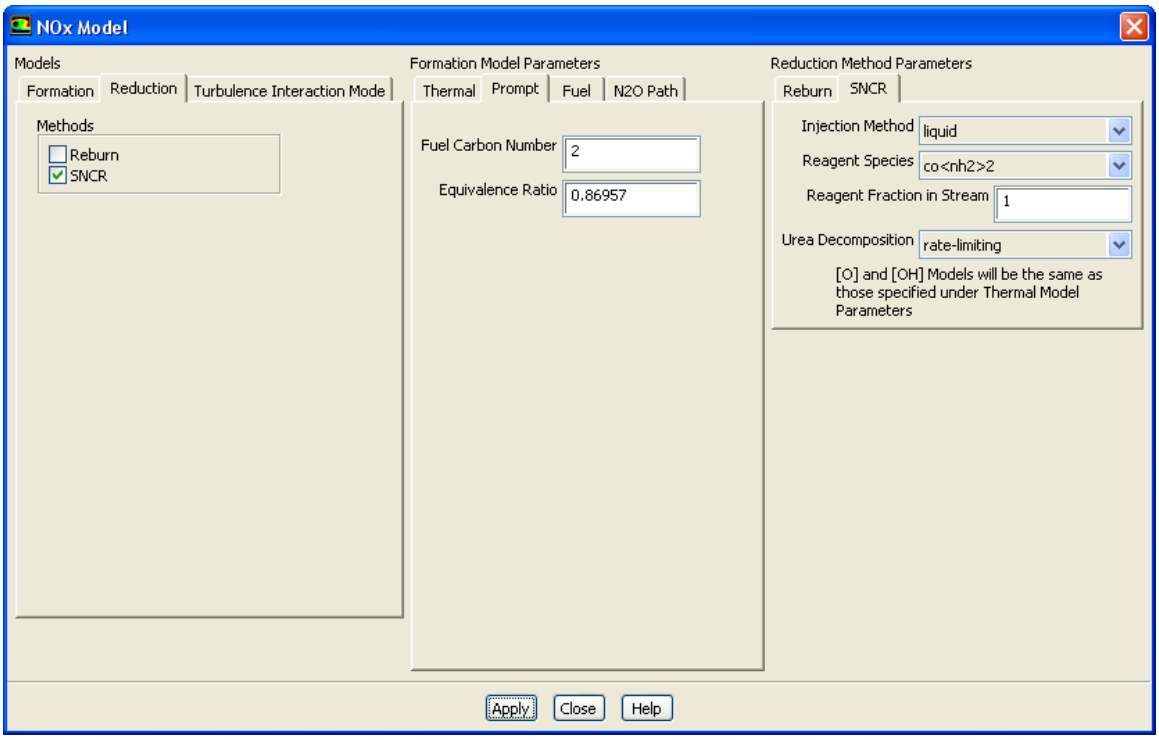

Figure 21.1.4: The NO_x Dialog Box Displaying the SNCR Reduction Method

Then click the SNCR tab under Reduction Method Parameters, where you can choose from the following options:

- To have ammonia or urea included as a gas-phase pollutant species from the injection locations, select gaseous in the Injection Method drop-down list.

  If you plan to select this option for NO_x postprocessing, then you must also include ammonia or urea as a gas-phase species. Additionally, you will need to specify the mass fraction of ammonia or urea at the respective inlet for the SNCR injection. You must include this set of inputs prior to the main ANSYS FLUENT combustion calculation.

- To have ammonia included as a liquid-phase pollutant species from the injection locations, select liquid in the Injection Method drop-down list. If urea is injected as a liquid solution, then select liquid in the Injection Method drop-down list. Note that you must activate the DPM model with urea or ammonia included as a material.

  If you plan to select this option for NO_x postprocessing, then you must include NH_3 as both a gas-phase and liquid-phase species. Additionally, you will need to specify

injection locations for liquid droplet ammonia particles and set gaseous ammonia as the evaporation species. You need to include this set of inputs in conjunction with the main ANSYS FLUENT combustion calculation.

Since urea is a subliming solid, and usually is injected as a solution, mixed in water, you have to define solid properties for urea under the Create/Edit Materials dialog box. We assume that the water evaporates before urea begins its subliming process. The sublimation process is modeled similar to the single rate devolatilization model of coal. You will supply the value for the sublimation rate (s^{-1}). You must specify the water content while defining the injection properties.

- Specify the SNCR Reagent Species as nh3 (ammonia) or co<nh2>2 (urea) in the drop-down list.

- When using the non-premixed combustion model with a liquid-phase reagent injection, enter a value in the Reagent Fraction in Stream to specify the mass fraction of the reagent in the reagent stream. The remaining mass fraction is assumed to be water. If you enabled a secondary stream in your PDF calculation, by default the secondary stream will act as the reagent stream. You can assign the primary stream as the reagent stream by using the text command that follows (enter 0 in response to the PDF Stream ID prompt that follows the Injection Method prompt):

  ```
  define/models/nox-parameters/nox-chemistry
  ```

- If the Reagent Species selected is co<nh2>2, then you will either accept the rate-limiting option for Urea Decomposition, or specify the NH3 Conversion value when selecting a user-specified Urea Decomposition.

  You will use the urea decomposition under the SNCR tab to define which of the two decomposition models is to be used. The first model (which is the default) is the rate-limiting decomposition model, as given in Table 13.1.3 in the separate Theory Guide. ANSYS FLUENT will then calculate the source terms according to the rates given in Table 13.1.3 in the separate Theory Guide. The second model is for the user who assumes urea decomposes instantly into ammonia and HNCO at a given proportion. In this case, you will specify the molar conversion fraction for ammonia, assuming that the rest of the urea is converted to HNCO. An example value is given above.

  The value for user-specified NH_3 conversion is the mole fraction of NH_3 in the mixture of NH_3 and HNCO that is instantly created from the reagent injection. In this case, there is no urea source because all of reagent is assumed to convert to both NH_3 and HNCO, instantly.

Setting Turbulence Parameters

If you want to take into account turbulent fluctuations (as described in Section 13.1.9: NOx Formation in Turbulent Flows in the separate Theory Guide) when you compute the specified NO_x formation (thermal, prompt, and/or fuel, with or without reburn), define the turbulence parameters in the Turbulence Interaction Mode tab.

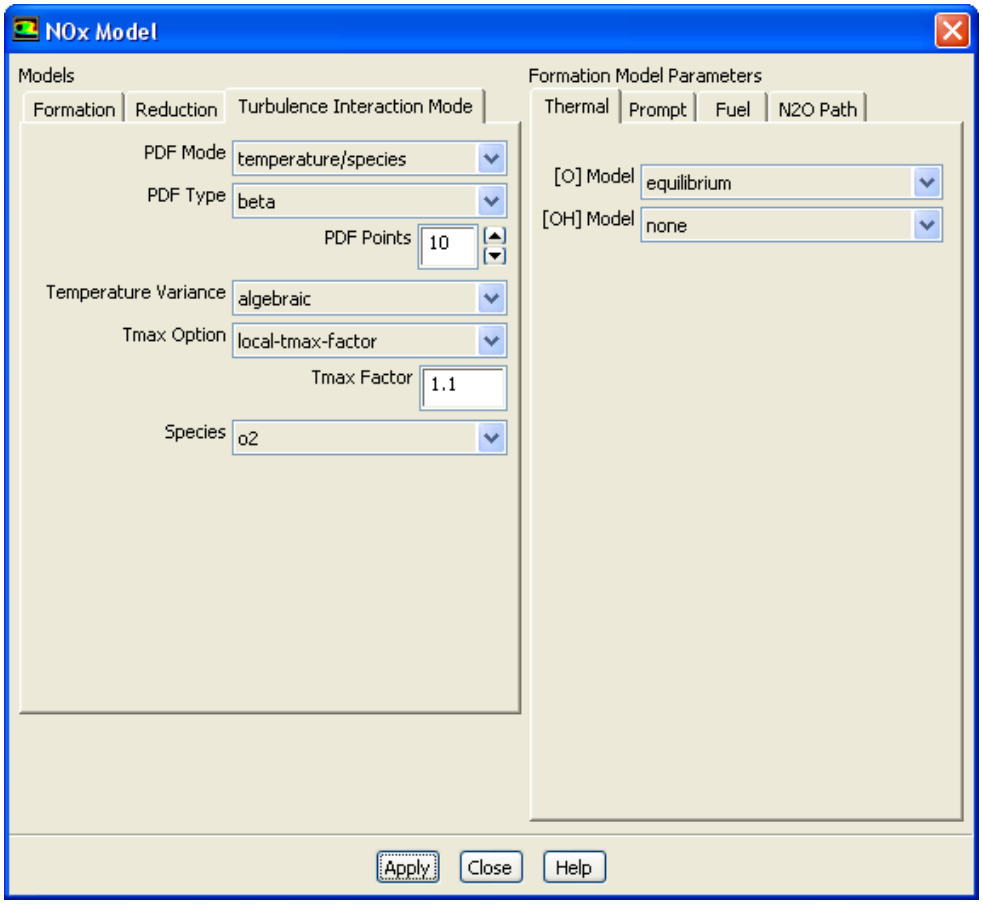

Figure 21.1.5: The NOx Model Dialog Box and the Turbulence Interaction Mode Tab

Select one of the options in the PDF Mode drop-down list in the Turbulence Interaction Mode tab:

- Select temperature to take into account fluctuations of temperature.
- Select temperature/species to take into account fluctuations of temperature and mass fraction of the species selected in the Species drop-down list (which appears when you select this option).

- (non-premixed and partially premixed combustion calculations only) Select mixture fraction to take into account fluctuation in the mixture fraction(s).

When modeling the formation of other pollutants along with NO_x, you should compare the selections made in the PDF Mode drop-down lists in the Turbulence Interaction Mode group boxes of the NOx Model dialog box and the Turbulence Interaction Mode group boxes of the SOx Model and Soot Model dialog boxes. If mixture fraction is selected in any of these dialog boxes, then it must be selected in all of the others as well.

The mixture fraction option is available only if you are using either the non-premixed or partially premixed combustion model to model the reacting system. If you use the mixture fraction option, the instantaneous temperatures and species concentrations are taken from the PDF look-up table as a function of mixture fraction and enthalpy and the instantaneous NO_x rates are calculated at each cell. The PDF used for convoluting the instantaneous NO_x rates is the same as the one used to compute the mean flow-field properties. For example, for single-mixture fraction models the beta PDF is used, and for two-mixture fraction models, the beta or the double delta PDF can be used. The PDF for mixture fraction is calculated from the values of mean mixture fraction and variance at each cell, and the instantaneous NO_x rates are convoluted with the mixture fraction PDF to yield the mean rates in turbulent flow.

If you selected temperature or temperature/species for the PDF Mode, you should define the following parameters in the Turbulence Interaction Mode tab:

PDF Type allows you to specify the shape of the PDF, which is then integrated to obtain mean rates for the temperature and (if you selected temperature/species for the PDF Mode) the species. If you select beta, the PDF will be modeled using Equation 13.1-107 in the separate Theory Guide. If you select gaussian, the PDF will be modeled using Equation 13.1-110 in the separate Theory Guide.

PDF Points allows you to specify the number of points used to integrate the beta or Gaussian function in Equation 13.1-104 or Equation 13.1-105 in the separate Theory Guide on a histogram basis. The default value of 10 will yield an accurate solution with reasonable computation time. Increasing this value may improve accuracy, but will also increase the computation time.

Temperature Variance allows you to specify the form of transport equation that is solved to calculate the temperature variance. The default selection is algebraic, which is an approximate form of the transport equation (see Equation 13.1-113 in the separate Theory Guide). You have the option of selecting transported to instead solve Equation 13.1-112 in the separate Theory Guide. Though the transported form is more exact, it is also more expensive computationally.

21.1.2 Solution Strategies

To solve for NO_x products, perform the following steps:

- (optional) If the discrete phase model (DPM) is activated (by turning on the Interaction with Continuous Phase) to run with the NO_x model, then set the Number of Continuous Phase Iterations per DPM Iteration to 0 such that no DPM iterations are performed as the NO_x case is being solved.
- In the Equations dialog box of the Solutions Controls task page, turn off the solution of all variables except species NO (and HCN, NH_3, or N_2O, based on the model selected).

  Solution Controls ⟶ Equations...
- Also in the Solution Controls task page, set a suitable value for the NO (and HCN, NH_3, or N_2O, if appropriate) under-relaxation. A value of 0.95 is suggested, although lower values may be required for certain problems (i.e., if convergence cannot be obtained, try a lower under-relaxation value).
- In the Residual Monitors dialog box, decrease the convergence criterion for NO (and HCN, NH_3, or N_2O, if appropriate) to 10^{-6}.

  Monitors ⟶ Residuals ⟶ Edit...
- Perform calculations until convergence (i.e., until the NO (and HCN, NH_3, or N_2O, if solved) species residuals are below 10^{-6}) to ensure that the NO and HCN or NH_3 concentration fields are no longer evolving.

  Run Calculation

i When you begin iterating with the NO_x model enabled, ANSYS FLUENT may report that the solution has converged after the first iteration. This is due to the lack of significant levels of pollutants in the solution. You can force ANSYS FLUENT to continue iterating by repeated iteration requests. Once pollutants appear in the solution, ANSYS FLUENT will continue iterating on its own until a steady solution is achieved.