*CHEMISTRY

The keyword *CHEMISTRY is used to access chemistry databases that include Chemkin-based descriptions of a chemical model, as well as to select a method of solving the model. The keyword cards in this section are defined in alphabetical order:

*CHEMISTRY_BATTERY†

*CHEMISTRY_COMPOSITION

*CHEMISTRY_CONTROL_0D

*CHEMISTRY_CONTROL_1D†

*CHEMISTRY_CONTROL_CSP

*CHEMISTRY_CONTROL_FULL

*CHEMISTRY_CONTROL_INFLATOR†

*CHEMISTRY_CONTROL_TBX

*CHEMISTRY_CONTROL_ZND†

*CHEMISTRY_DET_INITIATION†

*CHEMISTRY_INFLATOR_PROPERTIES†

*CHEMISTRY_MODEL

*CHEMISTRY_PATH

†: Card may be used only once in a given model

An additional option "_TITLE" may be appended to all *CHEMISTRY keywords. If this option is used, then an 80 character string is read as a title from the first card of that keyword's input. At present, LS-DYNA does not make use of the title. Inclusion of titles gives greater clarity to input decks.

The *CHEMISTRY_BATTERY card is only intended to be used in battery electrochemistry models that involve *BATTERY_... cards. Note that none of the comments below apply for this particular case.

*CHEMISTRY

In order to use one of the chemistry solvers, the input must include at least one *CHEMISTRY_MODEL card. For each spatial region containing a different chemical composition, at least one *CHEMISTRY_COMPOSITION card is required.

The *CHEMISTRY_CONTROL_0D card is intended to be used in a standalone fashion to verify the validity of a given chemistry model. This model includes the total number of species and all elementary reactions with their Arrhenius rate parameters. For instance, this solver could be used to check the induction time of the model.

The *CHEMISTRY_BLAST_INITIATION, *CHEMISTRY_CONTROL_1D, *CHEMISTRY_DET_INITIATION, and *CHEMISTRY_CONTROL_ZND cards are intended to provide a one-dimensional initialization to a 2D or 3D chemically-reacting flow.

In order to perform a full, general purpose chemistry calculation in 2D or 3D, the *CHEMISTRY_CONTROL_FULL card should be used.

The *CHEMISTRY_CONTROL_CSP card is an option for reducing the number of species and reactions that are used in a general purpose chemistry calculation. Other reduction mechanisms are planned for the future.

An airbag inflator model is available with *CHEMISTRY_CONTROL_INFLATOR along with *CHEMISTRY_INFLATOR_PROPERTIES and a chemistry model that is referenced via three chemical compositions. This involves zero-dimensional modeling, with pyrotechnic inflator, and cold and hot flow hybrid inflator options.

The *CHEMISTRY_CONTROL_TBX card is intended for use only in a stochastic particle model, where the *STOCHASTIC_TBX_PARTICLES card is used.

*CHEMISTRY_BATTERY

Purpose: For the battery electrochemistry solver (*BATTERY), this card identifies the files that define a Chemkin chemistry model for use with that solver.

Battery Reaction and Species Input File Card (Chemkin-compatible).

Card 1	1	2	3	4	5	6	7	8
Variable	FILE1							
Type	A							

Thermodynamics Database File Card.

Card 2	1	2	3	4	5	6	7	8
Variable	FILE2							
Type	A							

Transport Properties Database File Card.

Card 3	1	2	3	4	5	6	7	8
Variable	FILE3							
Type	A							

VARIABLE	DESCRIPTION
FILE1	Name of the file containing the Chemkin-compatible input
FILE2	Name of the file containing the chemistry thermodynamics database
FILE3	Name of the file containing the chemistry transport properties database

*CHEMISTRY_COMPOSITION

Purpose: Provide a general way to specify a chemical composition via a list of species mole numbers in the context of a Chemkin database model.

Card 1	1	2	3	4	5	6	7	8
Variable	ID	MODELID						
Type	I	I						
Default	none	none						

Species List Card. Provide as many cards as necessary. This input ends at the next keyword ("*") card.

Card 2	1	2	3	4	5	6	7	8
Variable	MOLFR	SPECIES						
Type	F	A						
Default	none	none						

VARIABLE	DESCRIPTION
ID	A unique identifier among all chemistry compositions
MODELID	Identifier of a Chemkin-compatible chemistry model (see *CHEMISTRY_MODEL)
MOLFR	The number of moles corresponding to the species named in the SPECIES field. But, if used with a *STOCHASTIC_TBX_PARTICLES card, it is the molar concentration of the species (in units of moles/[length]^3, where [length] is the user's length unit).
SPECIES	The Chemkin-compatible name of a chemical species that is defined in the chemistry model identified by MODELID (see *CHEMISTRY_MODEL)

*CHEMISTRY_CONTROL_0D

Purpose: Performs a zero-dimensional isotropic chemistry calculation that operates standalone (does not call the CESE solver). This is for ISOBARIC or ISOCHORIC cases.

Card 1	1	2	3	4	5	6	7	8
Variable	ID	COMPID	SOLTYP	PLOTDT	CSP_SEL			
Type	I	I	I	F	I			
Default	none	none	none	1.0e-6	0			
Remarks					1			

Card 2	1	2	3	4	5	6	7	8
Variable	DT	TLIMIT	TIC	PIC	RIC	EIC		
Type	F	F	F	F	F	F		
Default	none	none	none	none	none	none		

CSP Parameters Card. Include cards for each chemical species in the following format when CSP_SEL.GT.0. This input ends at the next keyword ("*") card.

Card 3	1	2	3	4	5	6	7	8
Variable	AMPL	YCUT						
Type	F	F						
Default	none	none						

VARIABLE	DESCRIPTION
ID	Identifier for this 0D computation.

VARIABLE	DESCRIPTION
COMPID	Chemical composition identifier of composition to use.
SOLTYP	Type of 0D calculation: EQ.1: Isochoric EQ.2: Isobaric
PLOTDT	Simulation time interval for output both to the screen and to the isocom.csv file. This file can be loaded into LS-PREPOST for curve plotting using the x-y plot facility.
CSP_SEL	CSP solver option: EQ.0: Do not use the CSP solver, and ignore the AMPL and YCUT parameters (default). GT.0: Use the CSP solver, with the AMPL and YCUT parameters.
DT	Initial time step
TLIMIT	Time limit for the simulation
TIC	Initial temperature
PIC	Initial pressure
RIC	Initial density
EIC	Initial internal energy
AMPL	Relative accuracy for the mass fraction of a chemical species in the Chemkin input file.
YCUT	Absolute accuracy for the mass fraction of a chemical species in the Chemkin input file.

Remarks:

1. If CSP_SEL.GT.0, then instead of using the full chemistry solver, the computational singular perturbation (CSP) method solver is used.

*CHEMISTRY_CONTROL_1D

Purpose: Loads a previously-computed one-dimensional detonation. It is then available for use in the CESE solver for initializing a computation. In the product regions, this card overrides the initialization of the *CESE_INITIAL_CHEMISTRY_… cards.

Card 1	1	2	3	4	5	6	7	8
Variable	ID	XYZD	DETDIR	CSP_SEL				
Type	I	F	I	I				
Default	none	none	none	0				
Remarks				1				

One-Dimensional Solution LSDA Input File Card.

Card 2	1	2	3	4	5	6	7	8
Variable	FILE							
Type	A							

CSP Parameters Card Include cards for each chemical species in the following format when CSP_SEL > 0. This input ends at the next keyword ("*") card.

Card 3	1	2	3	4	5	6	7	8
Variable	AMPL	YCUT						
Type	F	F						
Default	none	none						

VARIABLE	DESCRIPTION
ID	Identifier for this one-dimensional detonation solution.
XYZD	Position of the detonation front in the DETDIR direction.

VARIABLE	DESCRIPTION
DETDIR	Detonation propagation direction EQ.1: x EQ.2: y EQ.3: z
CSP_SEL	CSP solver option: EQ.0: Do not use the CSP solver, and ignore the AMPL and YCUT parameters (default). GT.0: Use the CSP solver, with the AMPL and YCUT parameters.
FILE	Name of the LSDA file containing the one-dimensional solution.
AMPL	Relative accuracy for the mass fraction of a chemical species in the chemkin input file.
YCUT	Absolute accuracy for the mass fraction of a chemical species in the chemkin input file.

Remarks:

1. If CSP_SEL > 0, then instead of using the full chemistry solver, the computational singular perturbation (CSP) method solver is used.

*CHEMISTRY_CONTROL_CSP

Purpose: Computes reduced chemistry for a specified Chemkin chemistry model using the Computational Singular Perturbation (CSP) method. This card can be used for general-purpose chemical reaction calculations.

Card 1	1	2	3	4	5	6	7	8
Variable	ID	IERROPT						
Type	I	I						
Default	none	none						

CSP Parameters Card. Include cards for each chemical species in the following format as indicated by the value of IERROPT. This input ends at the next keyword ("*") card.

Card 2	1	2	3	4	5	6	7	8
Variable	AMPL	YCUT						
Type	F	F						
Default	none	none						

VARIABLE	DESCRIPTION
ID	Identifier for this computational singular perturbation solver.
IERROPT	Selector: EQ.0: AMPL and YCUT values for all chemical species are required. EQ.1: One CSP Parameter Card should be provided, and it will be used for all species.
AMPL	Relative accuracy for the mass fraction of a chemical species in the Chemkin input file.
YCUT	Absolute accuracy for the mass fraction of a chemical species in the Chemkin input file.

*CHEMISTRY_CONTROL_FULL

Purpose: Computes the full chemistry specified by a Chemkin chemistry model. This card can be used for general-purpose chemical reaction calculations.

Card 1	1	2	3	4	5	6	7	8
Variable	ID	ERRLIM	RHOMIN	TMIN				
Type	I	F	F	F				
Default	none	none	0.0	0.0				

VARIABLE	DESCRIPTION
ID	Identifier for this full chemistry calculation.
ERRLIM	Error tolerance for the full chemistry calculation.
RHOMIN	Minimum fluid density above which chemical reactions are computed.
TMIN	Minimum temperature above which chemical reactions are computed.

*CHEMISTRY_CONTROL_INFLATOR

Purpose: Provide the required properties of an inflator model for airbag inflation.

Card 1	1	2	3	4	5	6	7	8
Variable	MODEL	OUT_TYPE	TRUNTIM	DELT	PTIME			
Type	I	I	F	F	F			
Remarks	1	2,4						

Inflator Output Database File (an ASCII file) Card.

Card 2	1	2	3	4	5	6	7	8
Variable	FILE							
Type	A							

Densities for Condensed Species. Include as many cards as needed. This input ends at the next keyword ("*") card.

Card 3	1	2	3	4	5	6	7	8
Variable	DENSITY	Species Name						
Type	F	A						
Default	none	none						
Remark		3						

VARIABLE	DESCRIPTION
MODEL	Type of inflator model to compute. EQ.1: Pyrotechnic model EQ.2: Hybrid model with cold flow option in the gas chamber EQ.3: Hybrid model with heat flow in the gas chamber EQ.4: Hybrid model with heat flow in one additional gas chamber EQ.5: Hybrid model with heat flow in two additional gas chambers
OUT_TYPE	Selects the output file format that will be used in an airbag simulation. EQ.0: Screen output calibration output (see Remark 4) EQ.1: CESE compressible flow solver (default) EQ.2: ALE solver EQ.3: CPM solver (with 2nd-order expansion of C_p) EQ.4: CPM solver (with 4th-order expansion of C_p)
TRUNTIM	Total run time.
DELT	Delta(t) to use in the model calculation.
PTIME	Time interval for output of time history data to FILE.
FILE	Name of the ASCII file in which to write the time history data and other data output by the inflator simulation.
DENSITY	Density of a condensed-phase species present in the inflator.
Species Name	Chemkin-compatible name of a condensed-phase species.

Remarks:

1. If MODEL = 3, the solution of an elementary reaction system is required for the finite-rate chemistry in the gas chamber. For MODEL = 4 and 5, the condensed phase is computed only in the combustion chamber.

2. Output file includes all of the necessary thermodynamics variables and load curves for the species mass flow rate, temperature, and density curve. This will make it possible to generate the velocity curve which is required by each solver that carries out an airbag simulation.

3. At least one of these cards will be input if condensed-phase species are present during the propellant combustion. In this case, the user must specify each condensed-phase density. This density is then used to compute the volume fractions in both the combustion and gas chamber, where the energy equations are needed.

4. If OUT_TYPE = 0, the propellant information will be displayed on the screen, including total mass, remaining mass percentage, and mass burning rate versus time, and the calibration data will be saved in the output file, including the time versus pressure, temperature, total mass flow rate, and individual species mass fractions for all chambers. With this option, the user can quickly see the effect of changing the parameters on the first three *CHEMISTRY_INFLATOR_PROPERTIES cards.

*CHEMISTRY_CONTROL_TBX

Purpose: Specify a chemistry solver for use in conjunction with stochastic TBX particles. This is intended only for modeling the second phase of an explosion where the explosive has embedded metal (aluminum) particles that are too large to have burned in the first phase of the explosion.

This chemistry card points to a *CHEMISTRY_MODEL card (via IDCHEM) with its associated *CHEMISTRY_COMPOSITION cards to set up the initial conditions. That is, it establishes the spatial distribution of the species in the model.

It is assumed that there is no chemical reaction rate information in the chemistry model files. This is done since a special chemical reaction mechanism is implemented for TBX modeling. If particles other than solid aluminum particles are embedded in the explosive, then another burn model has to be implemented.

Surface Part Card. Card 1 format used when the PART keyword option is active**.**

Card 1	1	2	3	4	5	6	7	8
Variable	IDCHEM	USEPAR						
Type	I	I						
Default	none	1						

VARIABLE	DESCRIPTION
IDCHEM	Identifier for this chemistry solver.
USEPAR	Coupling flag indicating if a *STOCHASTIC_TBX_PARTICLES card is provided for this model: EQ.1: uses a *STOCHASTIC_TBX_PARTICLES card (default). EQ.0: does not use such a card.

*CHEMISTRY_CONTROL_ZND

Purpose: Compute the one-dimensional reduced chemistry of a ZND model. It is then used in the initialization of the chemistry part of the CESE solver. When this card is used, the *CESE_INITIAL_CHEMISTRY… cards must specify the progressive variable (degree of combustion) in the HIC field.

Card 1	1	2	3	4	5	6	7	8
Variable	ID							
Type	I							
Default	none							

Card 2	1	2	3	4	5	6	7	8
Variable	F	EPLUS	Q0	GAM	XYZD	DETDIR		
Type	F	F	F	F	F	I		
Default	none	none	none	none	none	none		

VARIABLE	DESCRIPTION
ID	Identifier for this full chemistry calculation
F	Overdriven factor
EPLUS	EPLUS parameter of the ZND model
Q0	Q0 parameter of the ZND model
GAM	GAM parameter of the ZND model
XYZD	Position of the detonation front in the DETDIR direction
DETDIR	Detonation propagation direction: EQ.1: X-direction EQ.2: Y-direction

VARIABLE	DESCRIPTION
	EQ.3: Z-direction

*CHEMISTRY_DET_INITIATION

Purpose: Performs a one-dimensional detonation calculation based upon a chemical composition and initial conditions. It is then available for use immediately in the CESE solver for initializing a computation, or it can be subsequently used by the *CHEMISTRY_CONTROL_1D card in a later run. In the product regions, this card overrides the initialization of the *CESE_INITIAL_CHEMISTRY… cards.

Card 1	1	2	3	4	5	6	7	8
Variable	ID	COMPID	NMESH	DLEN	CFL	TLIMIT	XYZD	DETDIR
Type	I	I	I	F	F	F	F	I
Default	none	none	none	none	none	none	none	none

LSDA Output File Card.

Card 2	1	2	3	4	5	6	7	8
Variable	FILE							
Type	A							

VARIABLE	DESCRIPTION
ID	Identifier for this one-dimensional detonation computation.
COMPID	Chemical composition identifier of composition to use.
NMESH	Number of equal-width elements in the one-dimensional domain.
DLEN	Length of the one-dimensional domain.
CFL	Time-step limiting factor.
TLIMIT	Time limit for the simulation
XYZD	Position of the detonation front in the DETDIR direction.
DETDIR	Detonation propagation direction (1 => X; 2 => Y; 3 => Z)

VARIABLE	DESCRIPTION
FILE	Name of the LSDA file in which to write the one-dimensional solution.

*CHEMISTRY_INFLATOR_PROPERTIES

Purpose: Provide the required properties of an inflator model.

Card 1	1	2	3	4	5	6	7	8
Variable	COMP_ID	PDIA	PHEIGHT	PMASS	TOTMASS			
Type	I	F	F	F	F			
Remarks	1	2	2					

Card 2	1	2	3	4	5	6	7	8
Variable	TFLAME	PINDEX	A0	TDELAY	RISETIME			
Type	F	F	F	F	F			
Default	none	none	none	none	None			

Combustion Chamber Parameter Card.

Card 3	1	2	3	4	5	6	7	8
Variable	COMP1ID	VOL1	AREA1	CD1	P1	T1	DELP1	DELTI
Type	I	F	F	F	F	F	F	F
Default	none	none	none	none	none	none	none	none

Gas Plenum Parameter Card.

Card 4	1	2	3	4	5	6	7	8
Variable	COMP2ID	VOL2	AREA2	CD2	P2	T2	DELP2	DELT2
Type	I	F	F	F	F	F	F	F
Default	none	none	none	none	none	none	none	none

Tank Parameter Card.

Card 5	1	2	3	4	5	6	7	8
Variable	COMP3ID	VOL3	P3	T3				
Type	I	F	F	F				
Default	none	none	none	none				

Gas Chamber 1 (Optional, see Remark 3) Card.

Card 6	1	2	3	4	5	6	7	8
Variable	COMP4ID	VOL4	AREA4	CD4	P4	T4	DELP4	DELT4
Type	I	F	F	F	F	F	F	F
Default	none	none	none	none	none	none	none	none

Gas Chamber 2 (Optional, see Remark 3) Card.

Card 7	1	2	3	4	5	6	7	8
Variable	COMP5ID	VOL5	AREA5	CD5	P5	T5	DELP5	DELT5
Type	I	F	F	F	F	F	F	F
Default	none	none	none	none	none	none	none	none

VARIABLE	DESCRIPTION
COMP_ID	Chemical composition identifier of the composition for the steady-state propellant combustion (see Remark 1).
PDIA	Propellant diameter (see Remark 2).
PHEIGHT	Propellant height (see Remark 2).
PMASS	Individual cylinder (or sphere) propellant mass.
TOTMASS	Total propellant mass.
TFLAME	Adiabatic flame (combustion) temperature.
PINDEX	Power of the pressure in rate of burn model.
A0	Steady-state constant.
TDELAY	Ignition time delay.
RISETIME	Rise time.
COMP1ID	Chemical composition identifier of composition to use in the combustion chamber.
VOL1	Volume of the combustion chamber.
AREA1	Area of the combustion chamber.
CD1	Discharge coefficient of the combustion chamber.
P1	Pressure in the combustion chamber.

VARIABLE	DESCRIPTION
T1	Temperature in the combustion chamber.
DELP1	Rupture pressure in the combustion chamber.
DELT1	Elapsed time for breaking the burst disk between the chambers
COMP2ID	Chemical composition identifier of composition to use in the gas plenum.
VOL2	Volume of the gas plenum.
AREA2	Area of the gas plenum.
CD2	Discharge coefficient of the gas plenum.
P2	Pressure in the gas plenum.
T2	Temperature in the gas plenum.
DELP2	Rupture pressure in the gas plenum.
DELT2	Elapsed time for breaking the burst disk between the chambers
COMP3ID	Chemical composition identifier of composition to use in the tank.
VOL3	Volume of the tank.
P3	Pressure in the tank.
T3	Temperature in the tank.
COMP4ID	Chemical composition identifier of composition to use in the additional (second) gas chamber.
VOL4	Volume of the second gas chamber.
P4	Pressure in the second gas chamber.
T4	Temperature in the second gas chamber.
DELP4	Rupture pressure in the second gas chamber.
DELT4	Elapsed time for breaking the burst disk between the first and second gas chambers
COMP5ID	Chemical composition identifier of composition to use in the additional (third) gas chamber.

VOL5	Volume of the third gas chamber.
P5	Pressure in the third gas chamber.
T5	Temperature in the third gas chamber.
DELP5	Rupture pressure in the third gas chamber.
DELT5	Elapsed time for breaking the burst disk between the second and third gas chambers

Remarks:

1. The propellant composition can be obtained by running a chemical equilibrium program such as NASA CEA, the CHEETAH code, or the PEP code. LSTC provides a modified version of the PEP code along with documentation for users; it is available upon request.

2. A spherical shape for the propellant particles can be chosen if an identical value for the diameter and height is given.

3. To simulate a 4 or 5 chamber inflator, an additional chamber card can be used. In these cases of the inflator models, the condensed phase species are limited to the combustion chamber only if involved in the propellant combustion.

*CHEMISTRY_MODEL

Purpose: Identifies the files that define a Chemkin chemistry model.

Card 1	1	2	3	4	5	6	7	8
Variable	MODELID	JACSEL	ERRLIM					
Type	I	I	F					
Default	none	1	1.0e-3					

Chemkin Input File Card.

Card 2	1	2	3	4	5	6	7	8
Variable	FILE1							
Type	A							

Thermodynamics Database File Card.

Card 3	1	2	3	4	5	6	7	8
Variable	FILE2							
Type	A							

Transport Properties Database File Card.

Card 4	1	2	3	4	5	6	7	8
Variable	FILE3							
Type	A							

VARIABLE	DESCRIPTION
MODELID	Identifier for this Chemkin-based chemistry model

VARIABLE	DESCRIPTION
JACSEL	Selects the form of the Jacobian matrix for use in the source term: EQ.1: Fully implicit (default) EQ.2: Simplified implicit
ERRLIM	Allowed error in element balance in a chemical reaction
FILE1	Name of the file containing the Chemkin-compatible input
FILE2	Name of the file containing the chemistry thermodynamics database
FILE3	Name of the file containing the chemistry transport properties database

*CHEMISTRY_PATH

Purpose: To specify one or more search paths to look for chemistry database files.

Include as many cards as needed. This input ends at the next keyword ("*") card.

Card 1	1	2	3	4	5	6	7	8
Variable	DIR							
Type	A							

VARIABLE	DESCRIPTION
DIR	Directory path to add to the search set.