

***STOCHASTIC**

The keyword *STOCHASTIC is used to describe the particles and numerical details for solving a set of stochastic PDEs. Currently, there are two types of stochastic PDE models in the code: a spray model and a model of embedded particles in TBX explosives. The keyword cards for using these models are:

***STOCHASTIC_SPRAY_PARTICLES**

***STOCHASTIC_TBX_PARTICLES**

An additional option “_TITLE” may be appended to all *STOCHASTIC 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.

*STOCHASTIC

*STOCHASTIC_SPRAY_PARTICLES

*STOCHASTIC_SPRAY_PARTICLES

Purpose: Specify particle and other model details for spray modeling using stochastic PDEs that approximate such processes. A pair of cards is required to specify the characteristics of each nozzle (cards 3 and 4 describe the first nozzle).

Card 1	1	2	3	4	5	6	7	8
Variable	INJDIST	IBRKUP	ICOLLDE	IEVAP	IPULSE	LIMPR	IDFUEL	
Type	I	I	I	I	I	I	I	
Default	1	none	none	0	none	none	1	

Card 2	1	2	3	4	5	6	7	8
Variable	RHOP	TIP	PMASS	PRTRTE	STRINJ	DURINJ		
Type	F	F	F	F	F	F		

Nozzle card 1: Provide as many pairs of nozzle cards 1 and 2 as necessary. This input ends at the next keyword ("*") card (following a nozzle card 2).

Card 3	1	2	3	4	5	6	7	8
Variable	XORIG	YORIG	ZORIG	SMR	VELINJ	DRNOZ	DTHNOZ	
Type	F	F	F	F	F	F	F	

Nozzle card 2: Provide as many pairs of nozzle cards 1 and 2 as necessary. This input ends at the next keyword ("*") card.

Card 4	1	2	3	4	5	6	7	8
Variable	TILTXY	TILTXZ	CONE	DCONE	ANOZ	AMPO		
Type	F	F	F	F	F	F		

VARIABLE	DESCRIPTION
INJDIST	Spray particle size distribution: EQ.1: uniform EQ.2: Rosin-Rammler (default) EQ.3: Chi-squared degree of 2 EQ.4: Chi-squared degree of 6
IBRKUP	Type of particle breakup model: EQ.0: off (no breakup) EQ.1: TAB EQ.2: KHRT
ICOLLDE	Turn collision modeling on or off
IEVAP	Evaporation flag: EQ.0: off (no evaporation) EQ.1: Turn evaporation on (see Remark 1)
IPULSE	Type of injection: EQ.0: continuous injection EQ.1: sine wave EQ.2: square wave
LIMPRT	Upper limit on the number of parent particles modeled in this spray. This is not used with the continuous injection case (IP-ULSE = 0).

STOCHASTIC**STOCHASTIC_SPRAY_PARTICLES**

VARIABLE	DESCRIPTION
IDFUEL	Selected spray liquid fuels: EQ.1: (Default), H ₂ O EQ.2: Benzene, C ₆ H ₆ EQ.3: Diesel # 2, C ₁₂ H ₂₆ EQ.4: Diesel # 2, C ₁₃ H ₁₃ EQ.5: Ethanol, C ₂ H ₅ OH EQ.6: Gasoline, C ₈ H ₁₈ EQ.7: Jet-A, C ₁₂ H ₂₃ EQ.8: Kerosene, C ₁₂ H ₂₃ EQ.9: Methanol, CH ₃ OH EQ.10: N-dodecane, C ₁₂ H ₂₆
RHOP	Particle density
TIP	Initial particle temperature.
PMASS	Total particle mass
PRTRTE	Number of particles injected per second for continuous injection.
STRINJ	Start of injection(s)
DURINJ	Duration of injection(s)
XORIG	X-coordinate of center of a nozzle's exit plane
YORIG	Y-coordinate of center of a nozzle's exit plane
ZORIG	Z-coordinate of center of a nozzle's exit plane
SMR	Sauter mean radius
VELINJ	Injection velocity
DRNOZ	Nozzle radius
DTHNOZ	Azimuthal angle (in degrees measured counterclockwise) of the injector nozzle from the j = 1 plane.

VARIABLE	DESCRIPTION
TILTXY	Rotation angle (in degrees) of the injector in the x-y plane, where 0.0 points towards the 3 o'clock position ($j = 1$ line), and the angle increases counterclockwise from there.
TILTXZ	Inclination angle (in degrees) of the injection in the x-z plane, where 0.0 points straight down, $x > 0.0$ points in the positive x direction, and $x < 0.0$ points in the negative x direction.
CONE	Spray mean cone angle (in degrees) for hollow cone spray; spray cone angle (in degrees) for solid cone spray.
DCONE	Injection liquid jet thickness in degrees.
ANOZ	Area of injector
AMP0	Initial amplitude of droplet oscillation at injector

Remarks:

- When IEVAP = 1, the keyword input file must be modified in a fashion similar to a chemistry problem. This is illustrated in a portion of an example keyword file below. That is, the following keywords need to be used, along with the inclusion of other chemistry-related files (i.e. evap.inp and the corresponding thermodynamics data file):

*CHEMISTRY_MODEL
 *CHEMISTRY_COMPOSITION
 *CHEMISTRY_CONTROL_FULL
 *CESE_INITIAL_CHEMISTRY

```

$ Setup stochastic particles
$ 
*STOCHASTIC_SPRAY_PARTICLES
$ injdist ibrkup icollide     ievap      ipulse      limpct      fuelid
      3          1          0          1          0       100000          1
$ rhop      tip pmass[Kg]      prtrte      str_inj      dur_inj
  1000.0      300.      0.01      1.0e7      0.0       10.0
$ the next card is needed for fireball position and max. particle velocity:
$ Xorig      Yorig      Zorig      SMR      Velinj      Drnoz      Dthnoz
  0.005      0.005      1.0e-5      5.0e-6     200.0      9.0e-5
$ TILTXY     TILTXZ      CONE      DCONE      ANOZ      AMP0
      0.0          0.0        15.0        15.0      2.5e-8        0.0
$ 
*CHEMISTRY_MODEL
$ model_id    jacsel      errlim
  
```

*STOCHASTIC

*STOCHASTIC_SPRAY_PARTICLES

```
          10           1       0.0
  evap.inp
  therm.dat
  tran.dat
$
*CHEMISTRY_COMPOSITION
$  comp_id   model_id
    11        10
$  molefra   Species
    1.0        O2
    3.76       N2
$
*$CHEMISTRY_CONTROL_FULL
$  sol_id    errlim
    5
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$ Set global initial conditions for fluid
$
*CESE_INITIAL_CHEMISTRY
$  sol_id   comp_id
    5        11
$INITIAL CONDITIONS
$    uic      vic      wic      ric      pic      tic      hic
  0.0      0.0      0.0      1.2    101325.    300.0      0.0
```

***STOCHASTIC_TBX_PARTICLES**

Purpose: Specify particle and other model details for stochastic PDEs that model embedded particles in TBX explosives. Note that the components listed on the corresponding ***CHEMISTRY_COMPOSITION** card are in terms of molar concentrations of the species (in units of moles/[length]³, where [length] is the user's length unit).

For further information on the theory of the TBX model that has been implemented, a document on this topic can be found at this URL:

<https://lsdyna.ansys.com/cese-cfd-documentation/>

Card 1	1	2	3	4	5	6	7	8
Variable	PCOMB	NPRCL	MXCNT	PMASS	SMR	RHOP	TICP	T_IGNIT
Type	I	I	I	F	F	F	F	F
Default	0	none	none	none	none	none	none	none

Card 2	1	2	3	4	5	6	7	8
Variable	INITDST	AZIMTH	ALTITD	CPS/CVS	HVAP	EMISS	BOLTZ	
Type	I	F	F	F	F	F	F	
Default	1	none	none	none	none	optional	optional	
Remarks						1	1	

Card 3	1	2	3	4	5	6	7	8
Variable	XORIG	YORIG	ZORIG	XVEL	YVEL	ZVEL	FRADIUS	
Type	F	F	F	F	F	F	F	
Default	none	none	none	0.0	0.0	0.0	none	

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VARIABLE	DESCRIPTION
PCOMB	Particle combustion model: EQ.0: No burning EQ.1: K-model
NPRTCL	Initial total number of parent particles (discrete particles for calculation)
MXCNT	Maximum allowed number of parent particles (during the simulation)
PMASS	Total particle mass
SMR	Sort mean particle radius
RHOP	Particle density
TICP	Initial particle temperature
T_IGNIT	Particle ignition temperature
INITDST	Initial particle distribution: EQ.1: Spatially uniform EQ.2: Rosin-Rammler EQ.3: Chi-squared
AZIMTH	Angle in degrees from the x -axis in the xy -plane of the reference frame of the TBX explosive ($0 < \text{AZMITH} < 360$)
ALTITD	Angle in degrees from the z -axis of the reference frame of the TBX explosive ($0 < \text{ALTITD} < 180$)
CPS/CSV	Heat coefficient
HVAP	Latent heat of vaporization
EMISS	Particle emissivity
BOLTZ	Boltzmann coefficient
XORIG	x -coordinate of the origin of the initial reference frame of the TBX explosive

VARIABLE	DESCRIPTION
YORIG	y -coordinate of the origin of the initial reference frame of the TBX explosive
ZORIG	z -coordinate of the origin of the initial reference frame of the TBX explosive
XVEL	x -component of the initial particle velocity of the TBX explosive
YVEL	y -component of the initial particle velocity of the TBX explosive
ZVEL	z -component of the initial particle velocity of the TBX explosive
FRADIUS	Radius of the explosive area

Remarks:

1. **Radiation heat transfer.** If radiation heat transfer is being modeled, then EMISS and BOLTZ are required.

