FORMATION AND DECAY OF A DETONATION WAVE IN GAS – DSMC SIMULATION

Z. A. Walenta, K. Lener

PWSZ Jarosław

DIRECT MONTE - CARLO SIMULATION:

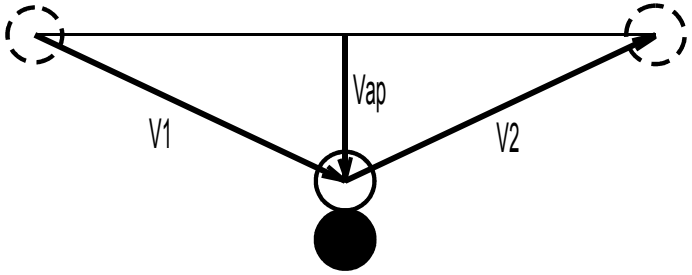
- GAS – ENSEMBLE OF MOLECULES MOVING FREELY IN SPACE, COLLIDING AMONG THEMSELVES, REFLECTING FROM THE WALLS.
- ONLY BINARY COLLISIONS OF MOLECULES OCCUR.
- CALCULATION AREA SPLIT INTO A NUMBER OF CELLS. ONLY MOLECULES FROM THE SAME CELL COLLIDE. THE PAIRS OF MOLECULES FOR COLLISIONS SELECTED AT RANDOM WITH ONE OF THE AVAILABLE ALGORITHMS (THE BALLOT – BOX ALGORITHM OF YANITSKIY USED IN THE PAPER)
- MOLECULES – HARD SPHERES (ASSUMED FOR SIMPLICITY OF CALCULATIONS)
- REFLECTIONS FROM WALLS – EITHER SPECULAR OR DIFFUSE.

MODEL OF A COMBUSTIBLE GAS:

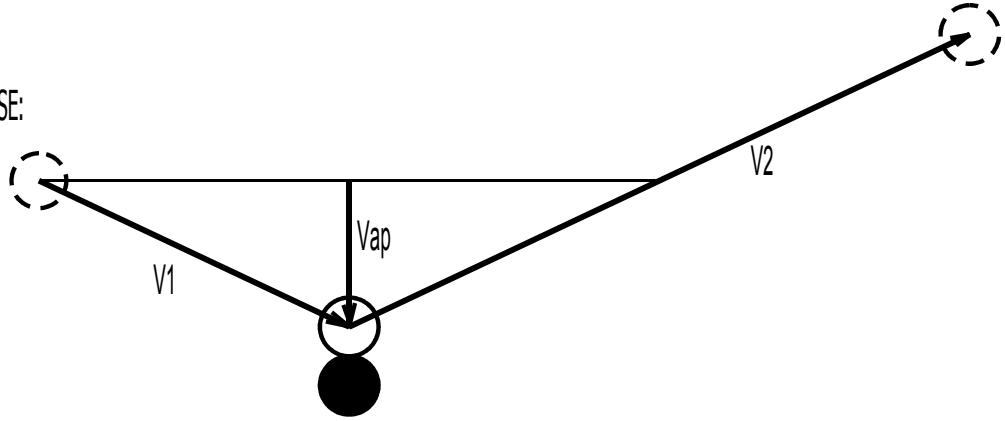
- SOME GAS MOLECULES CARRY „INTERNAL” ENERGY, RELEASED DURING COLLISIONS WITH OTHER MOLECULES AND TRANSFORMED INTO KINETIC ENERGY OF THEIR RELATIVE MOTION IF THE „VELOCITY OF APPROACH” EXCEEDS CERTAIN LEVEL
- ENERGY RELEASE OCCURS DURING THE FIRST COLLISION OF THIS KIND (NO DELAY), OR DURING SOME LATER COLLISION (DELAYED RELEASE)
- MOLECULE, WHICH LOST ITS „INTERNAL” ENERGY, MAY REGAIN IT IF IT COLLIDES WITH ANOTHER MOLECULE WITH SUFFICIENTLY HIGH „VELOCITY OF APPROACH” (THE INVERSE RACTION)

COLLISION OF TWO MOLECULES
IN REFERENCE FRAME CONNECTED TO ONE OF THEM

ELASTIC:



WITH ENERGY RELEASE:



V1 - relative velocity of the molecules before collision

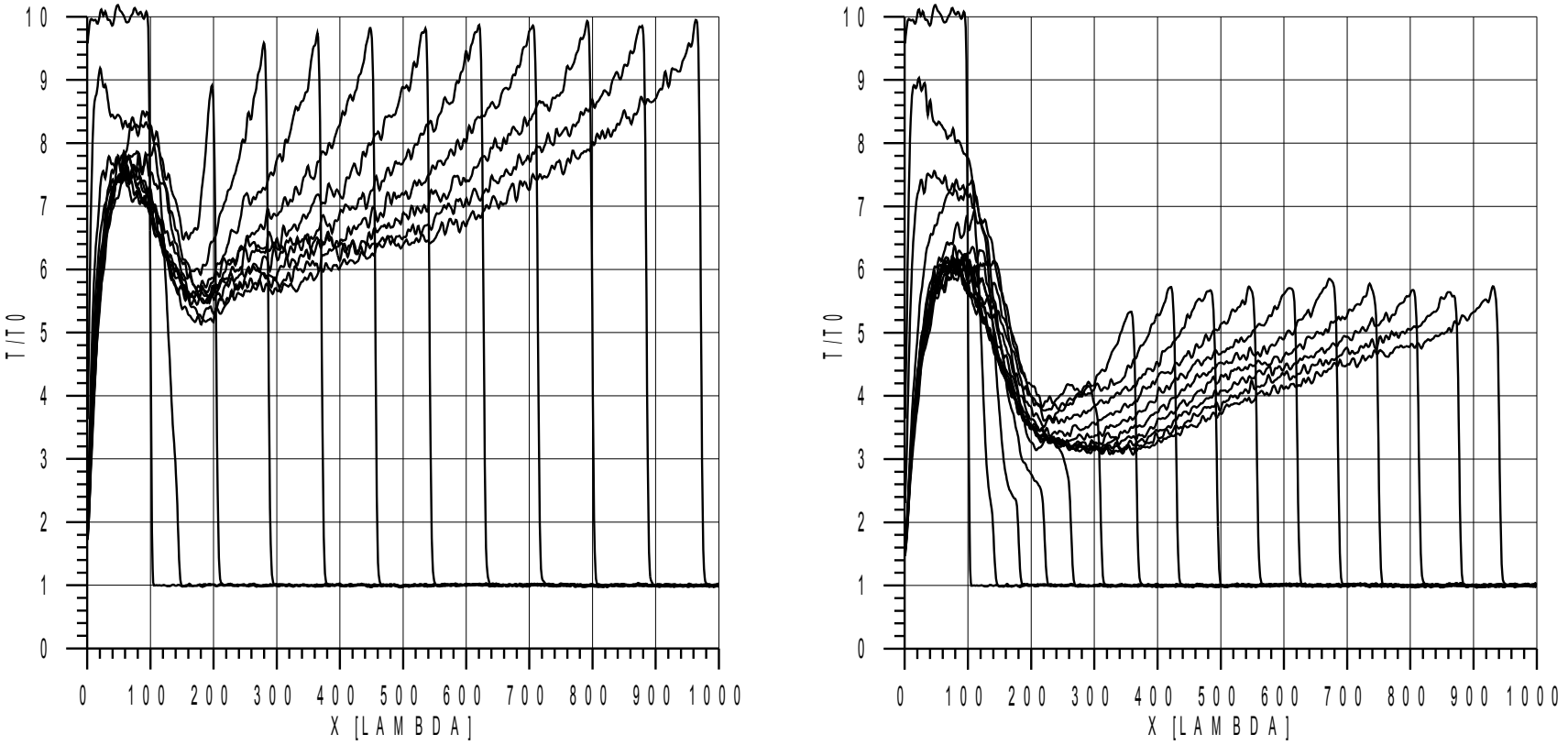
V2 - relative velocity after collision

Vap - "velocity of approach" of the molecules

DETAILS OF CALCULATION

- FLOW IN POSITIVE HALF–SPACE (1–DIMENSIONAL GEOMETRY) OR IN A PIPE 100 MEAN FREE PATHS DIAMETER (3–DIMENSIONAL GEOMETRY) INITIATED BY REMOVAL OF DIAPHRAGM SEPARATING DRIVER FROM DRIVEN GASES.
- CALCULATION AREA SPLIT INTO CELLS ONE MEAN FREE PATH (LAMBDA) LONG
- DRIVEN GAS CONTAINS 10, 20 OR 30 PER CENT OF MOLECULES CARRYING „INTERNAL" ENERGY.
- ENERGY RELEASED IN A SINGLE COLLISION INCREASES RELATIVE VELOCITY OF COLLIDING MOLECULES BY THE VALUE EQUAL TO 10 TIMES THE MOST PROBABLE MOLECULAR SPEED
- TO RELEASE THE „INTERNAL" ENERGY THE „VELOCITY OF APPROACH" MUST EXCEED THE VALUE 5.48 (IN SOME CASES 4.47) TIMES THE MOST PROBABLE MOLECULAR SPEED

1 – D GEOMETRY

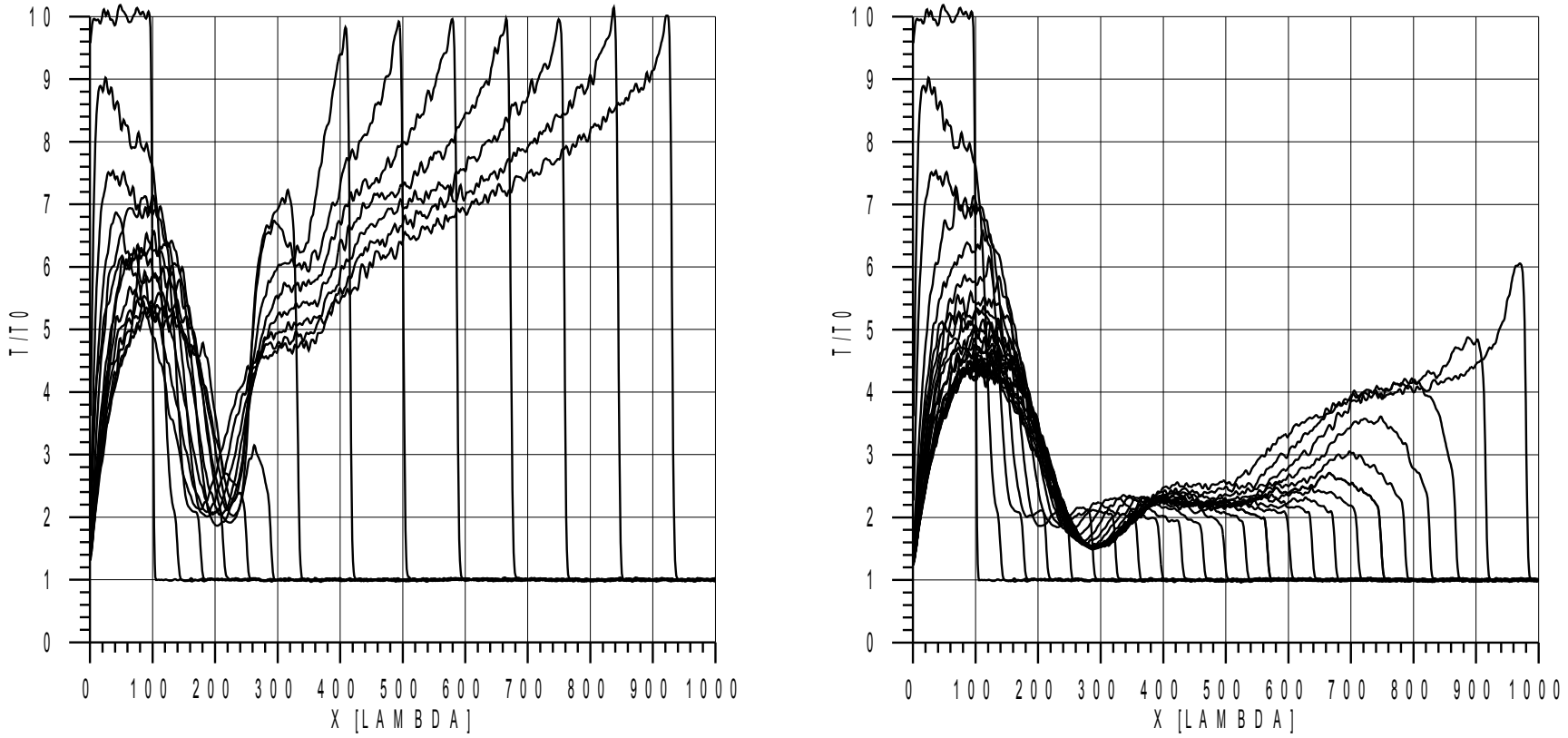


PLANE DETONATION WAVE – TEMPERATURE DISTRIBUTIONS

INITIATION BY SHOCK (Ms = 2) AND CONTACT WITH HOT DRIVER GAS
DRIVEN GAS CONTAINS 20 (LEFT) OR 10 (RIGHT) PER CENT OF „ENERGETIC” MOLECULES

T0 – INITIAL TEMPERATURE OF DRIVEN GAS, LAMBDA – INITIAL MEAN FREE PATH

1 – D GEOMETRY

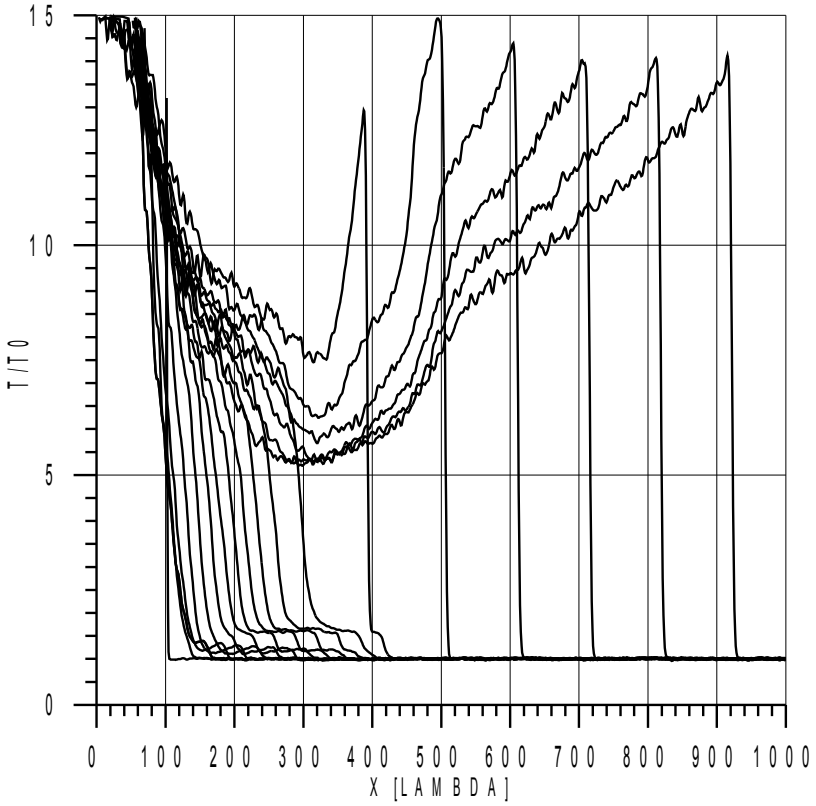


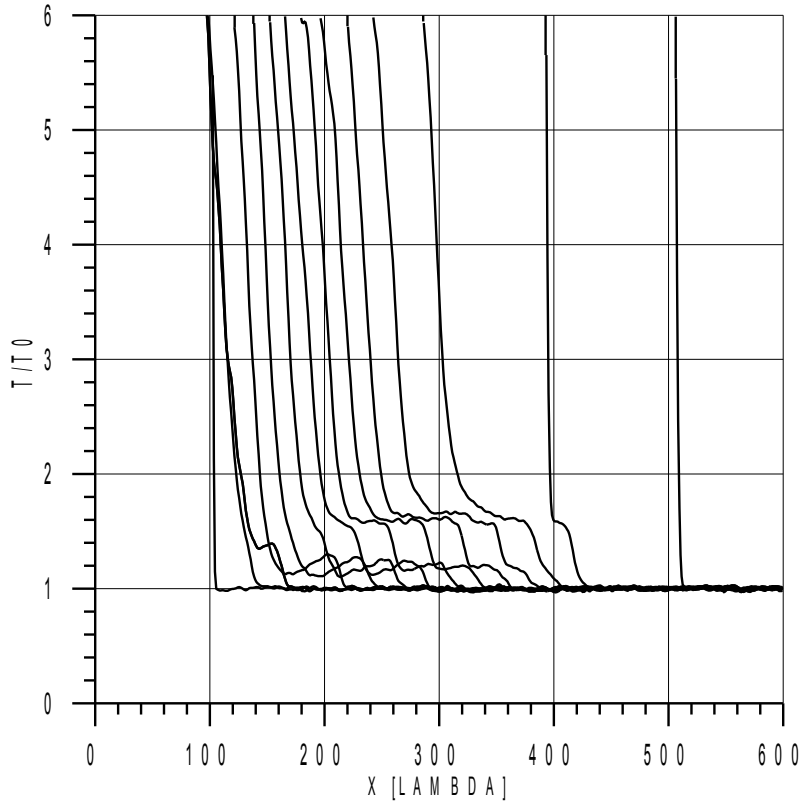
PLANE DETONATION WAVE – TEMPERATURE DISTRIBUTIONS

INITIATION BY SHOCK WAVE (Ms = 2) ONLY.
BETWEEN DRVER AND DRIVEN GASES – A BUFFER OF COLD, INERT GAS.
DRIVEN GAS CONTAINS 20 (LEFT) OR 10 (RIGHT) PER CENT OF „ENERGETIC” MOLECULES

T0 – INITIAL TEMPERATURE OF DRIVEN GAS, LAMBDA – INITIAL MEAN FREE PATH

1 – D GEOMETRY

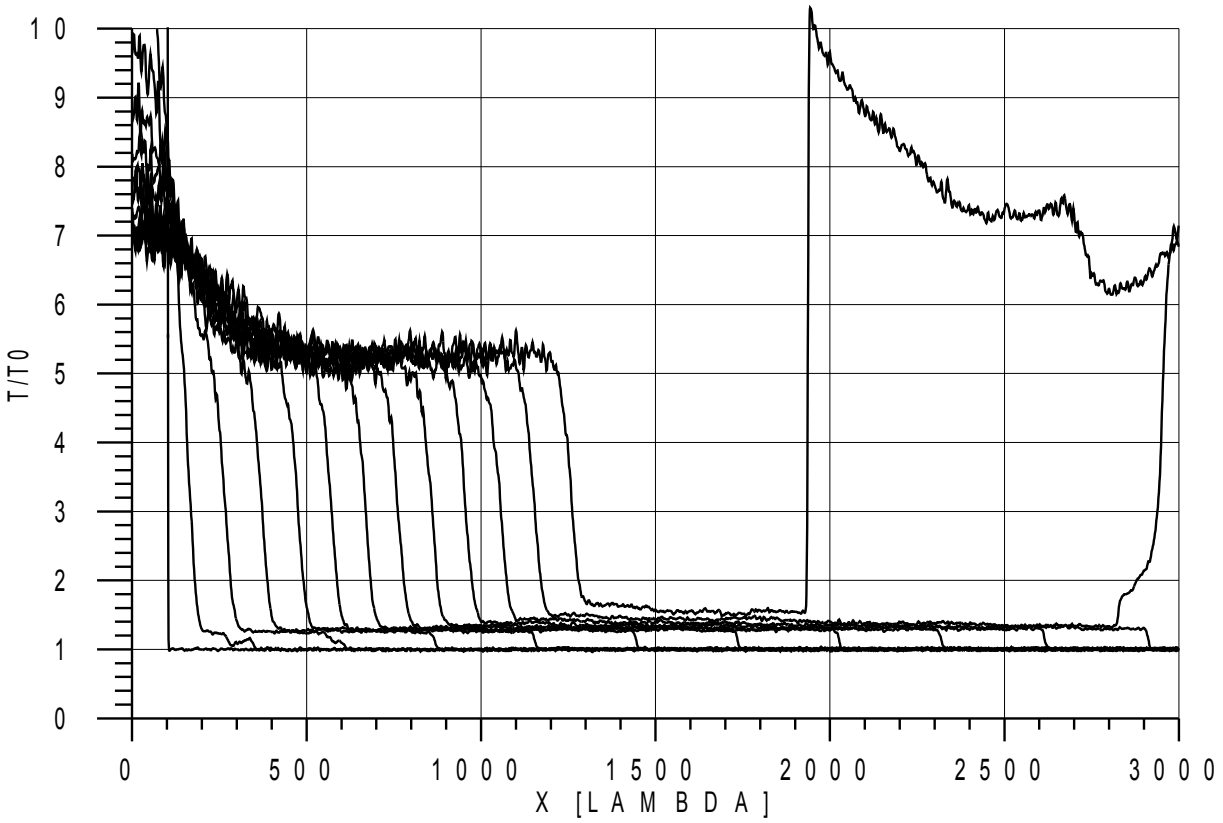




PLANE DETONATION WAVE – TEMPERATURE DISTRIBUTIONS

INITIATION BY CONTACT WITH HOT DRIVER GAS OF THE SAME PRESSURE AS DRIVEN GAS
DRIVEN GAS CONTAINS 30 PER CENT OF „ENERGETIC" MOLECULES
RIGHT – ENLARGED PART OF THE DIAGRAM SHOWN ON THE LEFT.
T0 – INITIAL TEMPERATURE OF DRIVEN GAS, LAMBDA – INITIAL MEAN FREE PATH

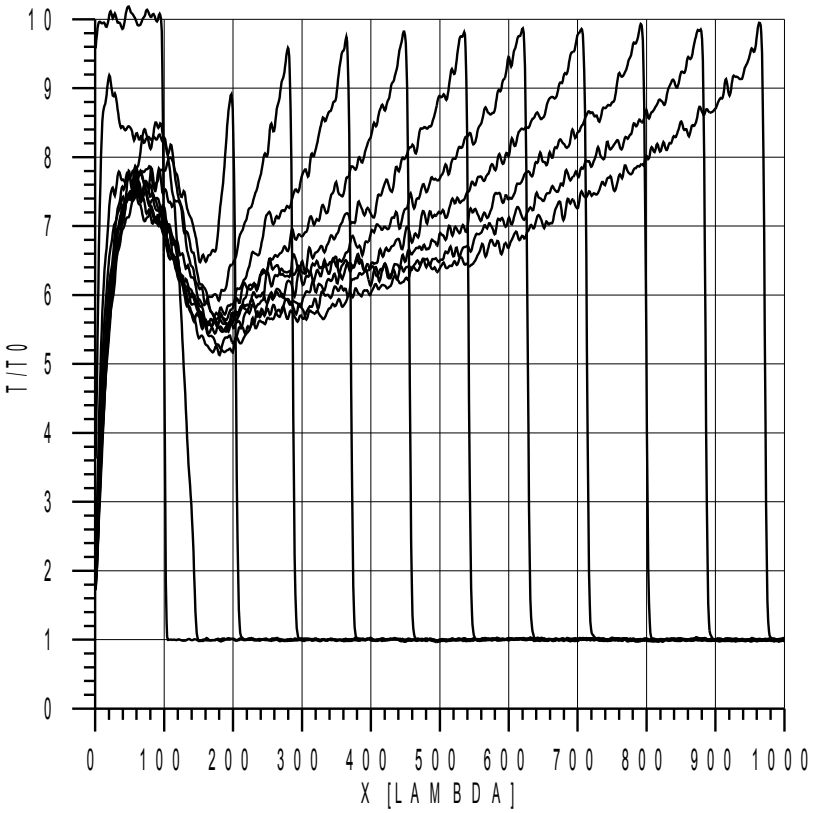
1 – D GEOMETRY

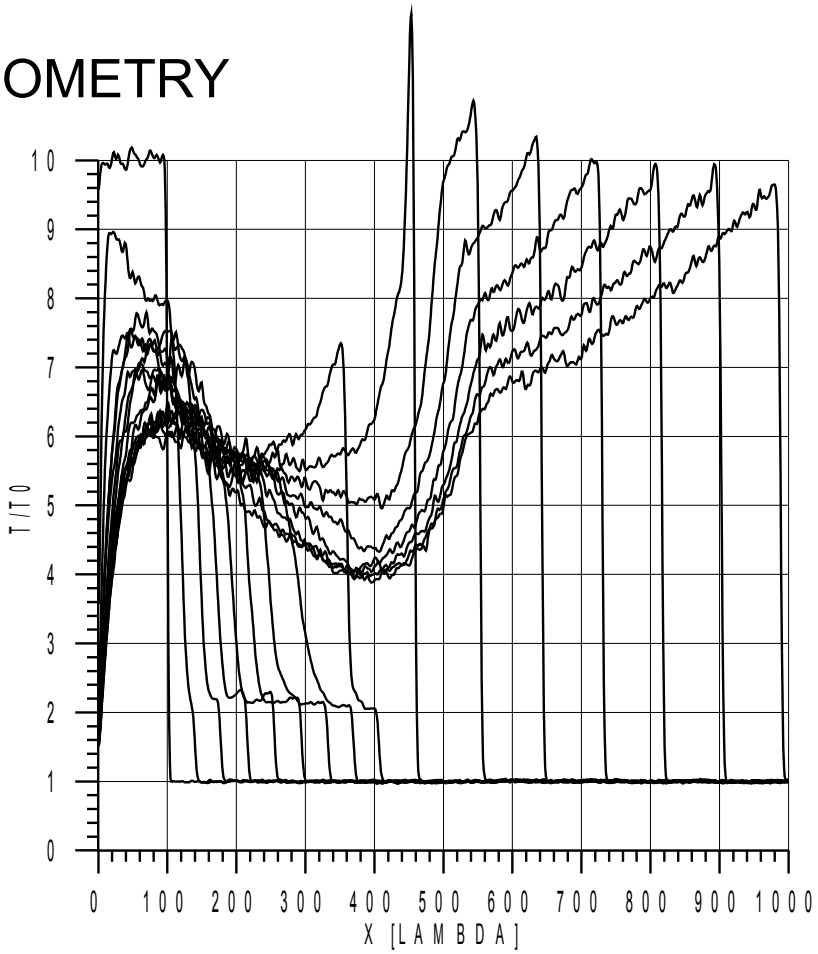


PLANE DETONATION WAVE – TEMPERATURE DISTRIBUTIONS

INITIATION BY CONTACT WITH HOT DRIVER GAS OF THE SAME PRESSURE AS DRIVEN GAS
DRIVEN GAS CONTAINS 20 PER CENT OF „ENERGETIC" MOLECULES
DETONATION DEVELOPS AFTER REFLECTION OF THE SHOCK FROM THE ENDWALL
T0 – INITIAL TEMPERATURE OF DRIVEN GAS, LAMBDA – INITIAL MEAN FREE PATH

1 – D GEOMETRY

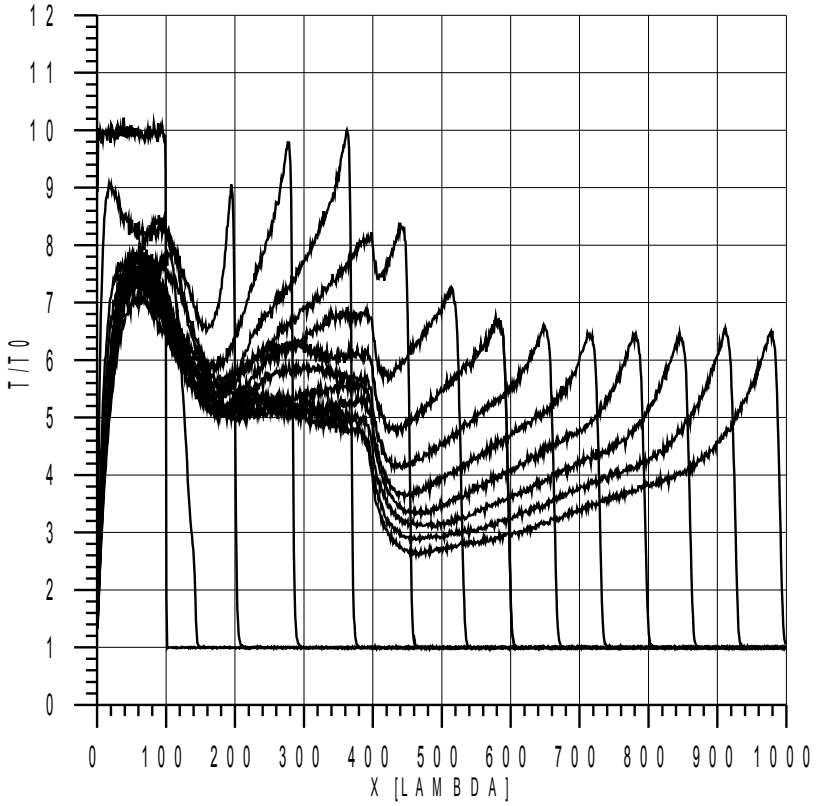


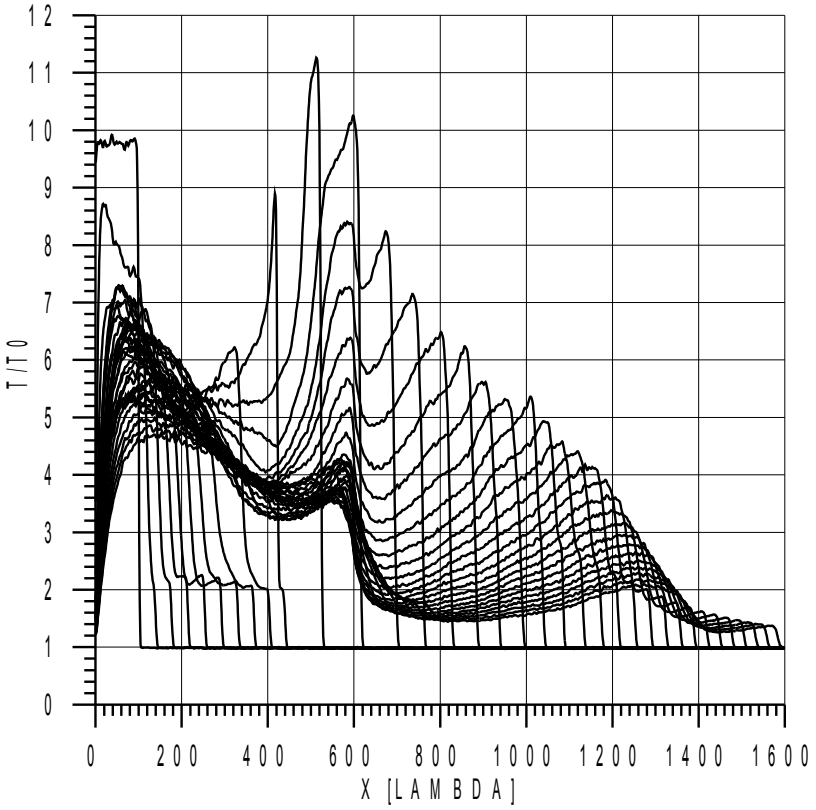


PLANE DETONATION WAVE – TEMPERATURE DISTRIBUTIONS

INITIATION BY SHOCK (Ms = 2) AND CONTACT WITH HOT DRIVER GAS
DRIVEN GAS CONTAINS 20 PER CENT OF „ENERGETIC" MOLECULES
LEFT – NO DELAY IN ENERGY RELEASE; RIGHT – ENERGY RELEASE IN 6-TH COLLISION
T0 – INITIAL TEMPERATURE OF DRIVEN GAS, LAMBDA – INITIAL MEAN FREE PATH

3 – D GEOMETRY





DETONATION WAVE IN A NARROW PIPE – TEMPERATURE DISTRIBUTIONS

INITIATION BY SHOCK (Ms = 2) AND CONTACT WITH HOT DRIVER GAS

DRIVEN GAS CONTAINS 20 PER CENT OF „ENERGETIC" MOLECULES

LEFT – NO DELAY IN ENERGY RELEASE; X < 400 – SPECULAR REFL., LATER – DIFFUSE

RIGHT – ENERGY RELEASE IN 6-TH COLLISION; X < 600 – SPECULAR REFLECTION

T0 – INITIAL TEMPERATURE OF DRIVEN GAS, LAMBDA – INITIAL MEAN FREE PATH

CONCLUSIONS

- DIRECT MONTE–CARLO SIMULATION TECHNIQUE – USEFUL FOR STUDYING DETONATION IN GASES, PARTICULARLY WHEN INFLUENCE OF WALLS IS IMPORTANT,
- THE PROPOSED MODEL OF „DETONATING GAS” MAKES IT POSSIBLE TO SIMULATE IN A SIMPLE WAY THE GAS PARAMETERS IMPORTANT FROM THE POINT OF VIEW OF DETONATION,
- THE FACTOR MOST IMPORTANT FOR DETONATION SEEMS TO BE THE ENERGY RELEASE – PRODUCT OF ENERGY RELEASED IN A SINGLE COLLISION AND FRACTION OF MOLECULES CARRYING THE „INTERNAL ENERGY”,
- THE OTHER IMPORTANT FACTORS ARE: DELAY IN THE ENERGY RELEASE AND THRESHOLD VELOCITY FOR ITS INITIATION,
- THE INVERSE REACTION APPEARS TO HAVE LITTLE INFLUENCE UPON DETONATION, PRESUMABLY BECAUSE THE MEDIUM IS FAR FROM THERMODYNAMIC EQUILIBRIUM AND COMBUSTION PROCEEDS VERY FAST,

CONCLUSIONS (2)

- IN CASE OF DETONATION PROPAGATING IN NARROW CHANNELS (E.G. IN DEVICES EXTINGUISHING DETONATION) THE IMPORTANT FACTOR IS KNUDSEN NUMBER – RATIO OF THE MEAN FREE PATH TO THE DIAMETER OF THE CHANNEL.