



BRITISH AMERICAN
TOBACCO

Nicotine Particle/Gas Phase Distribution Trends: Denuder Tube Studies

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PRESENTATION

- INTRODUCTION

- Objectives

- Denuder Tube Technology

- EQUIPMENT AND METHOD DEVELOPMENT

- Equipment Design

- Performance

- NICOTINE STUDIES

- Particle/Gas Equilibria

- SUMMARY AND CONCLUSIONS



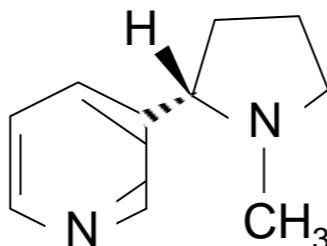
OBJECTIVES

1. To Examine the Influence of Humidity and Temperature on Nicotine Particle/Gas Phase Partitioning
2. To Compare Models that Estimate the Initial Fraction of Gas Phase Nicotine Exiting a Cigarette Filter

DENUnder TUBE TECHNOLOGY

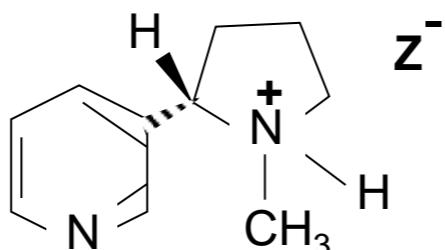
SMOKE NICOTINE: SPECIATION

Unprotonated Nicotine



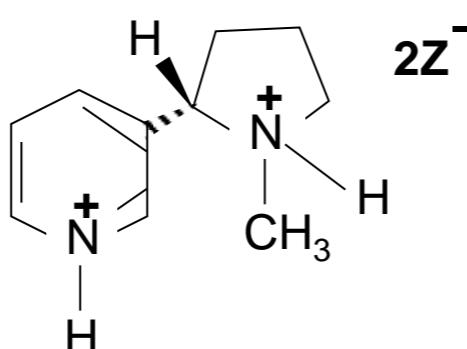
Aerosol Distribution: Particle and Gas Phases

Mono-Protonated Nicotine



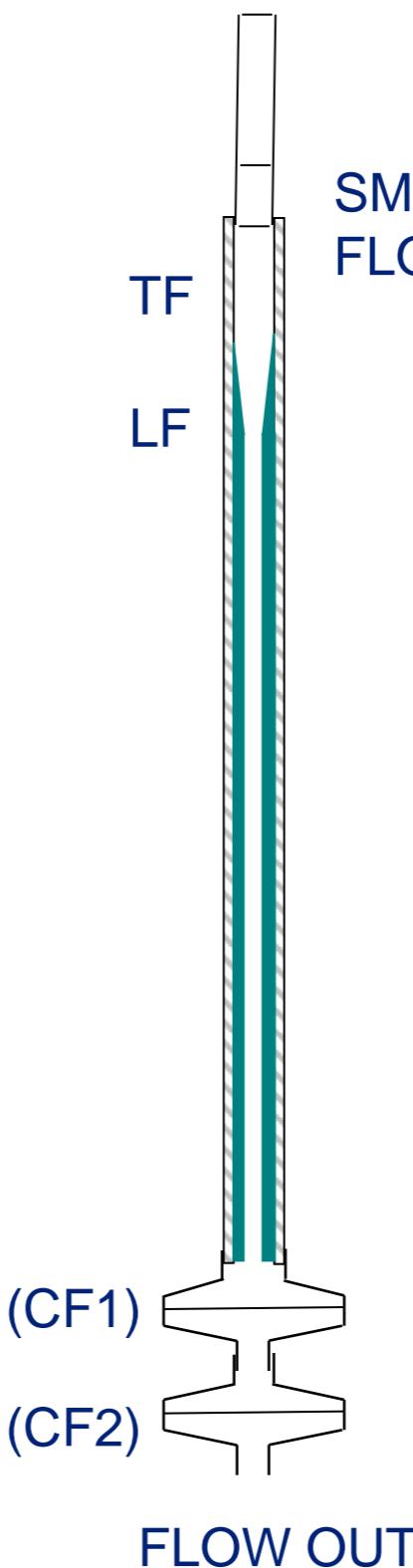
Aerosol Distribution: Particle Phase

Di-Protonated Nicotine (Negligible importance)



Aerosol Distribution: Particle Phase

Nicotine (N) Equilibria



DENUnder

TF Turbulent Flow

LF Laminar Flow

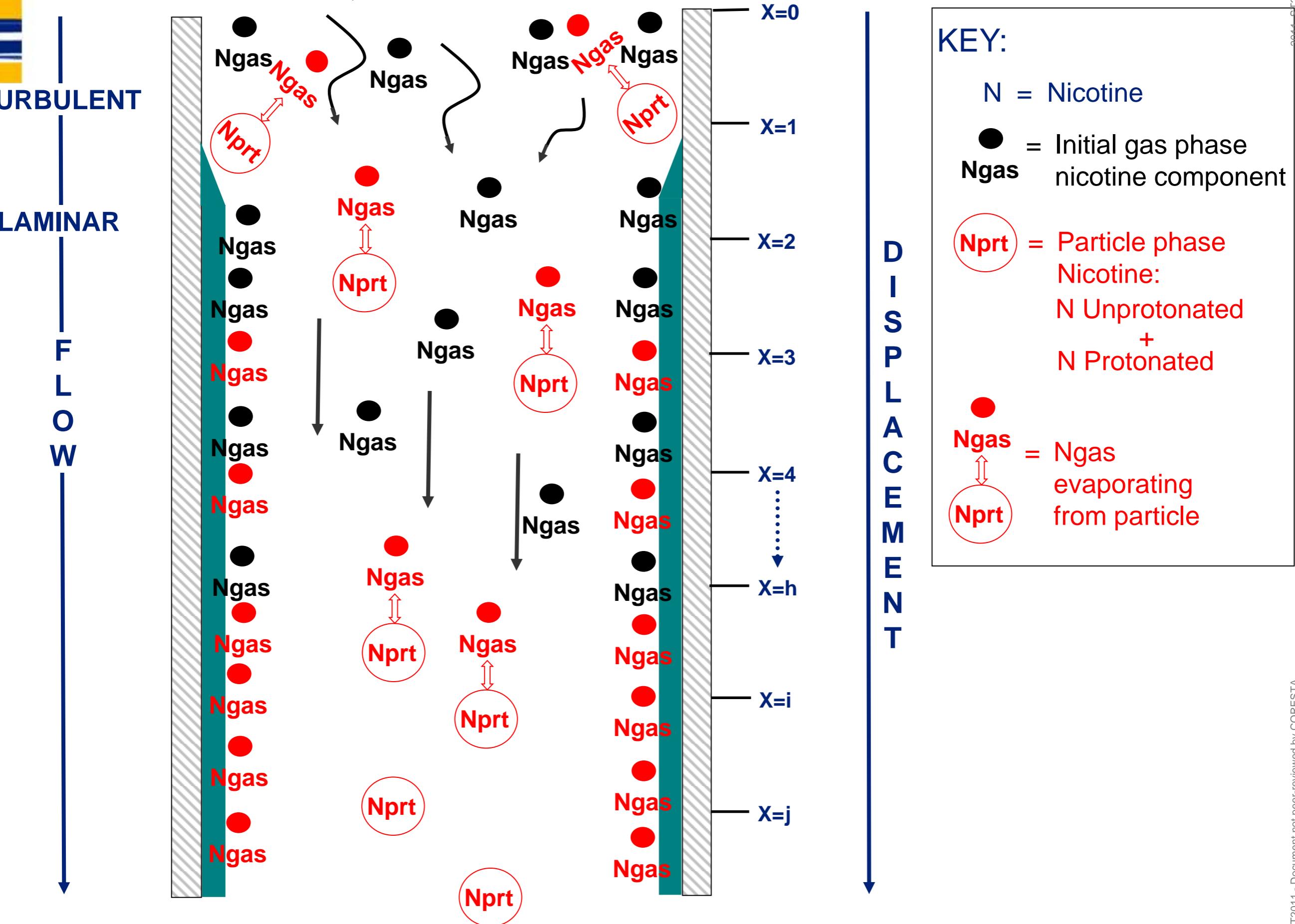
- Wall particle deposition minimal

SMOKE FLOW IN

NICOTINE:

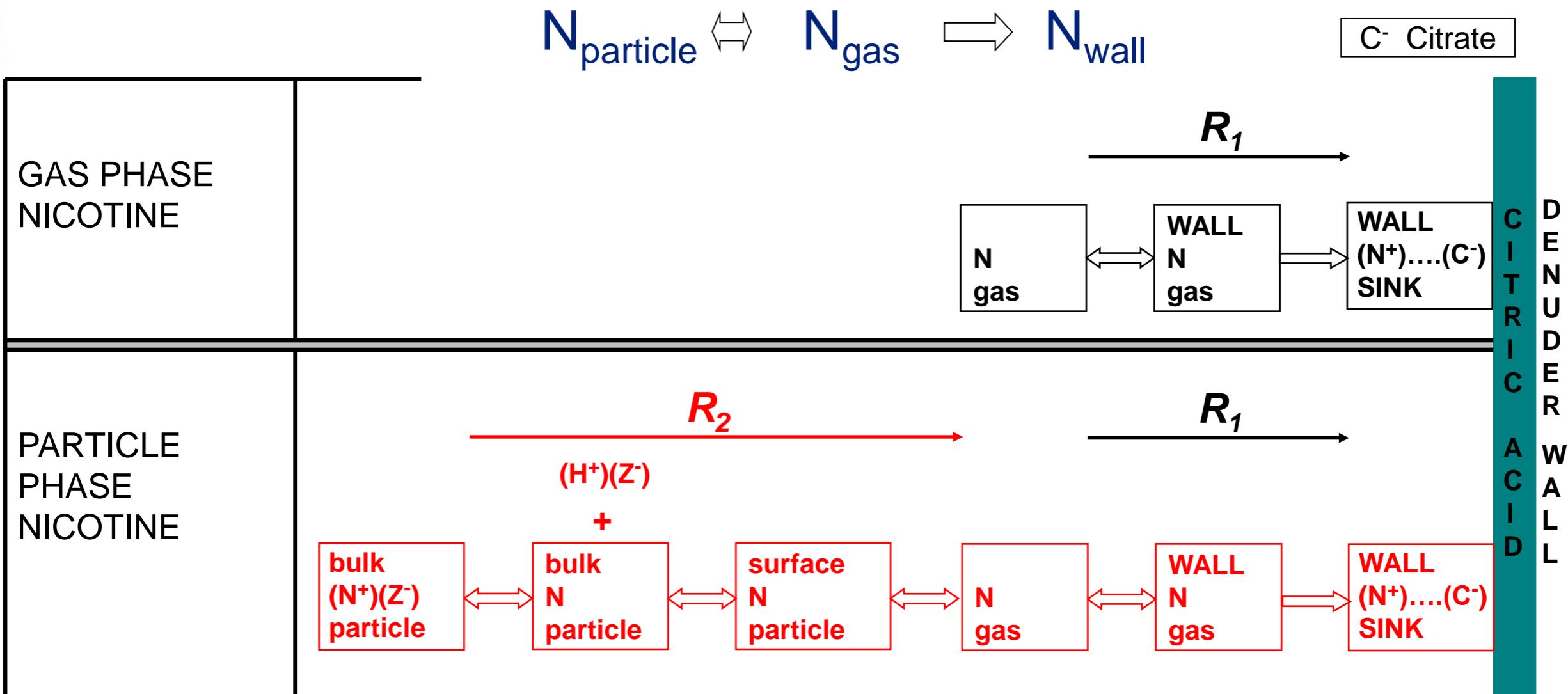
- Gas phase unprotonated nicotine removed at wall coating reactive 'sink' layer. Particle entrained unprotonated nicotine effuses from particles
- Unprotonated nicotine within particles evaporates and released - equilibria complex: gas phase nicotine trapped at wall as in (1)
- Particles flow through denuder with laminar flow streamlines
- Particles exit denuder and filtered
 - Cambridge Filter (CF1)
 - Cambridge Filter (CF2): citric acid impregnated

NICOTINE EQUILIBRIA



SMOKE NICOTINE EQUILIBRIA

Overall Nicotine (N) Equilibria Hypothesis



HYPOTHESIS

- Initial gas phase nicotine component diffuses to walls (rate R_1) and is removed
- Particle nicotine released into gas phase by evaporation and is removed similarly to (1). A series of physico-chemical principles influence evaporation rate from particles (rate R_2).
- When $R_1 \gg R_2$

initial denuder wall nicotine predominantly from initial gas phase nicotine

latter denuder wall nicotine predominantly from particle derived gas phase nicotine

EQUIPMENT DESIGN

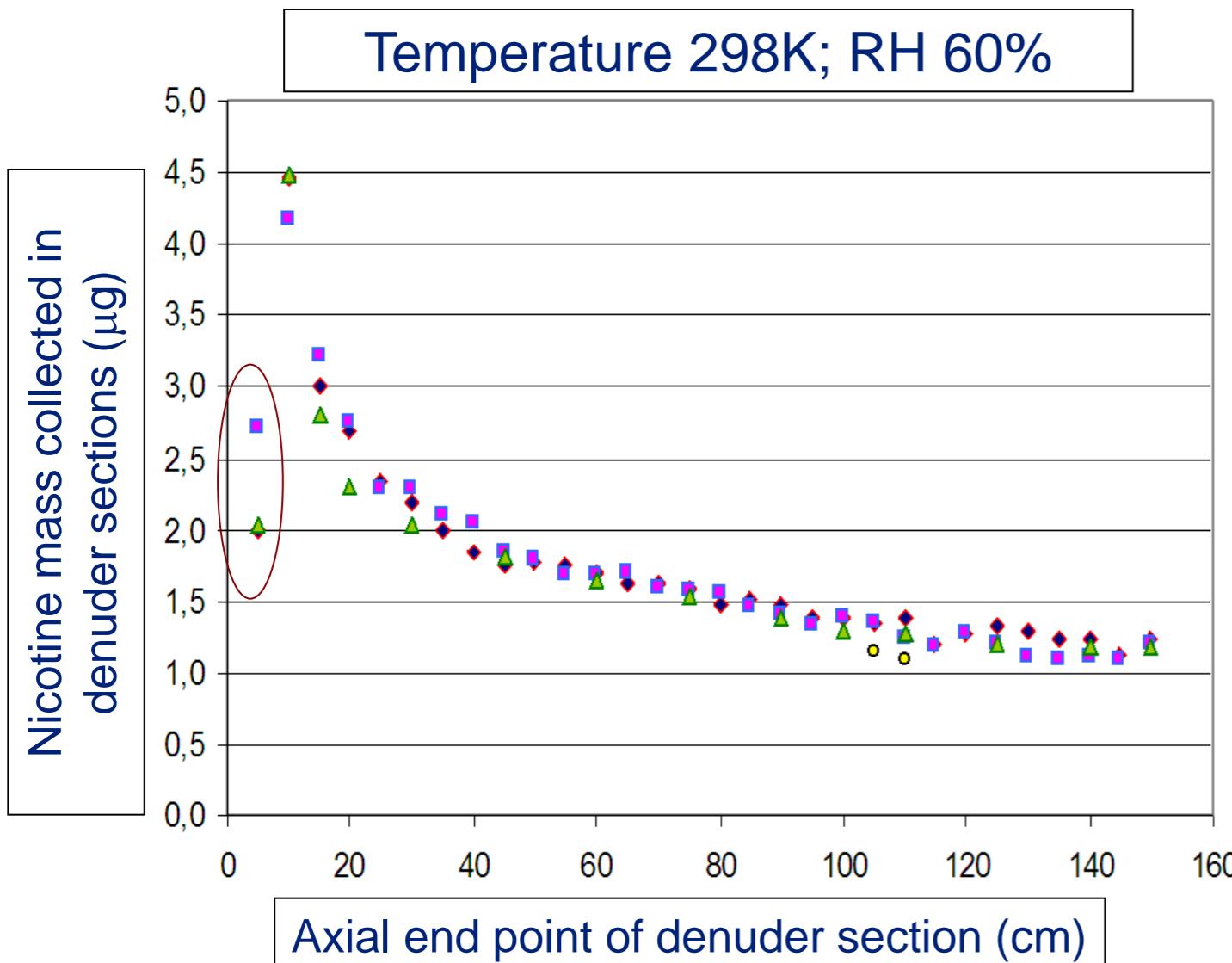


PERFORMANCE: REPEATABILITY

- Equipment/procedure presented at CORESTA Congress, Edinburgh 14 Sept 2010; SSPT15
- Robust & repeatable continuous draw technique
- Denuder: Operating Parameter Range

PARAMETER	CAPABILITY	UTILISED
Flow Rate ($\text{cm}^3 \text{s}^{-1}$)	0.2 - 17	5
Smoke Dilution (%)	0 - 50	Not utilised
RH (%)	20 - 80	30, 45, 60
Temperature ($^\circ\text{C}$ (K))	To 50 (323)	25 (298); 37 (310); 50 (323)

- First point anomaly: tip ventilation dependent



4 Replicates

Cigarette: 3R4F; 3 cigarettes smoked at 2cm length – 4 replicates

Denuder: 1.5m length; 0.8cm i.d.; citric-acid coating, first 5cm uncoated

Parameters: 298K; 60% RH; $5\text{cm}^3\text{s}^{-1}$

Exit: Cambridge filter plus backup citric acid impregnated Cambridge filter

NICOTINE STUDIES

PARTICLE/GAS EQUILIBRIA

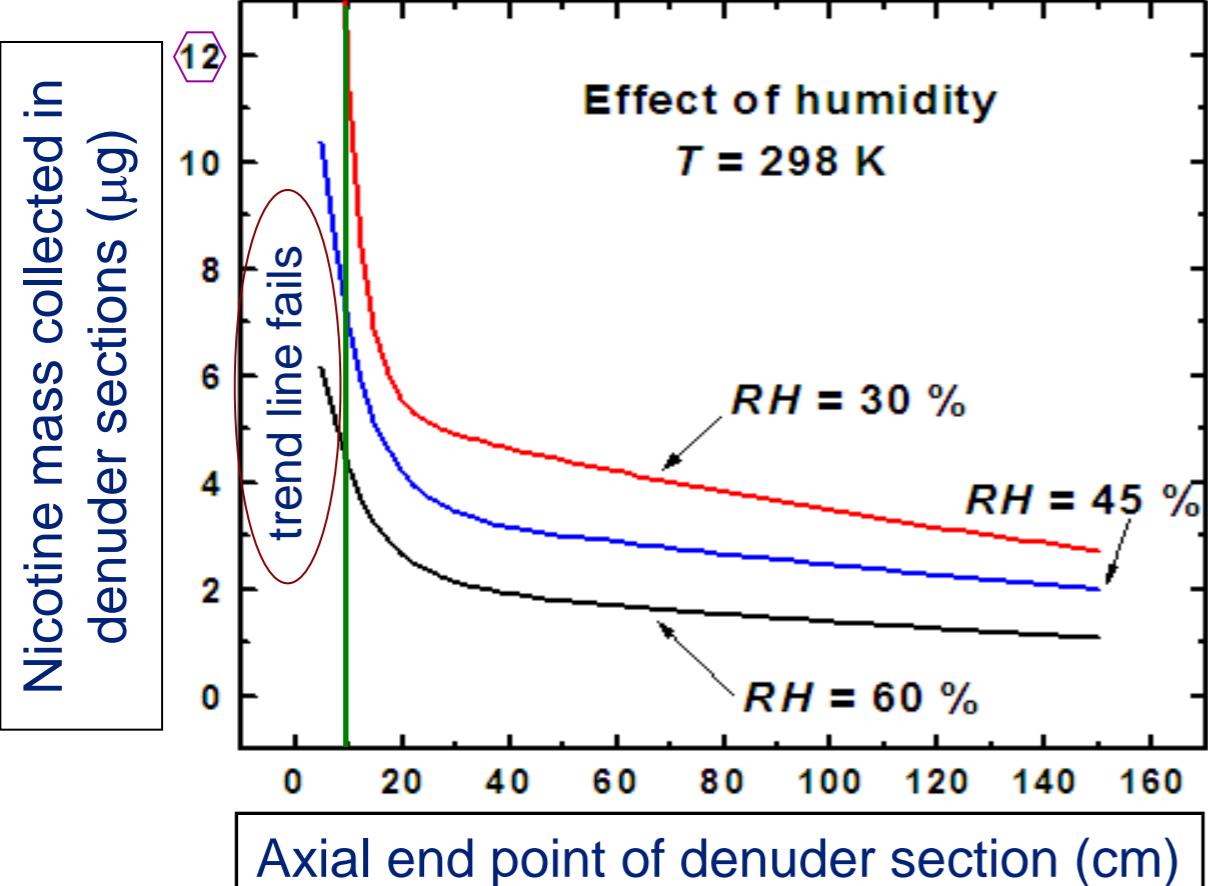
Influence of Smoking Environment RH and Denuder Temperature

DENUDER EXPERIMENTAL PARAMETERS

Denuder Temperature (K)	SMOKING ENVIRONMENT RH (%)		
	RH1 (%)	RH2 (%)	RH3 (%)
T1 298K	30	45	60
T2 310K	30	45	60
T3 323K	30	45	60

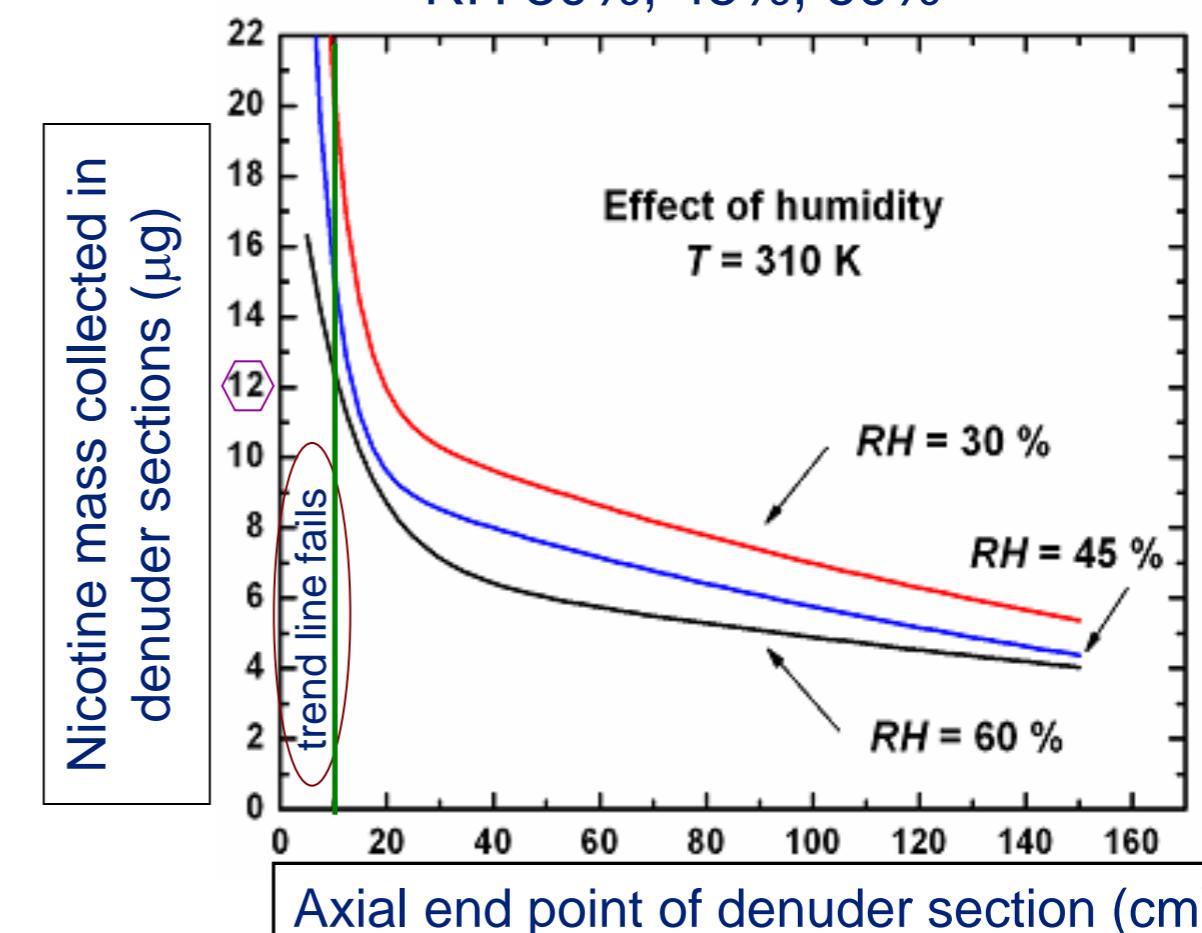
Composite Graph: T = 298K

RH 30%, 45%, 60%

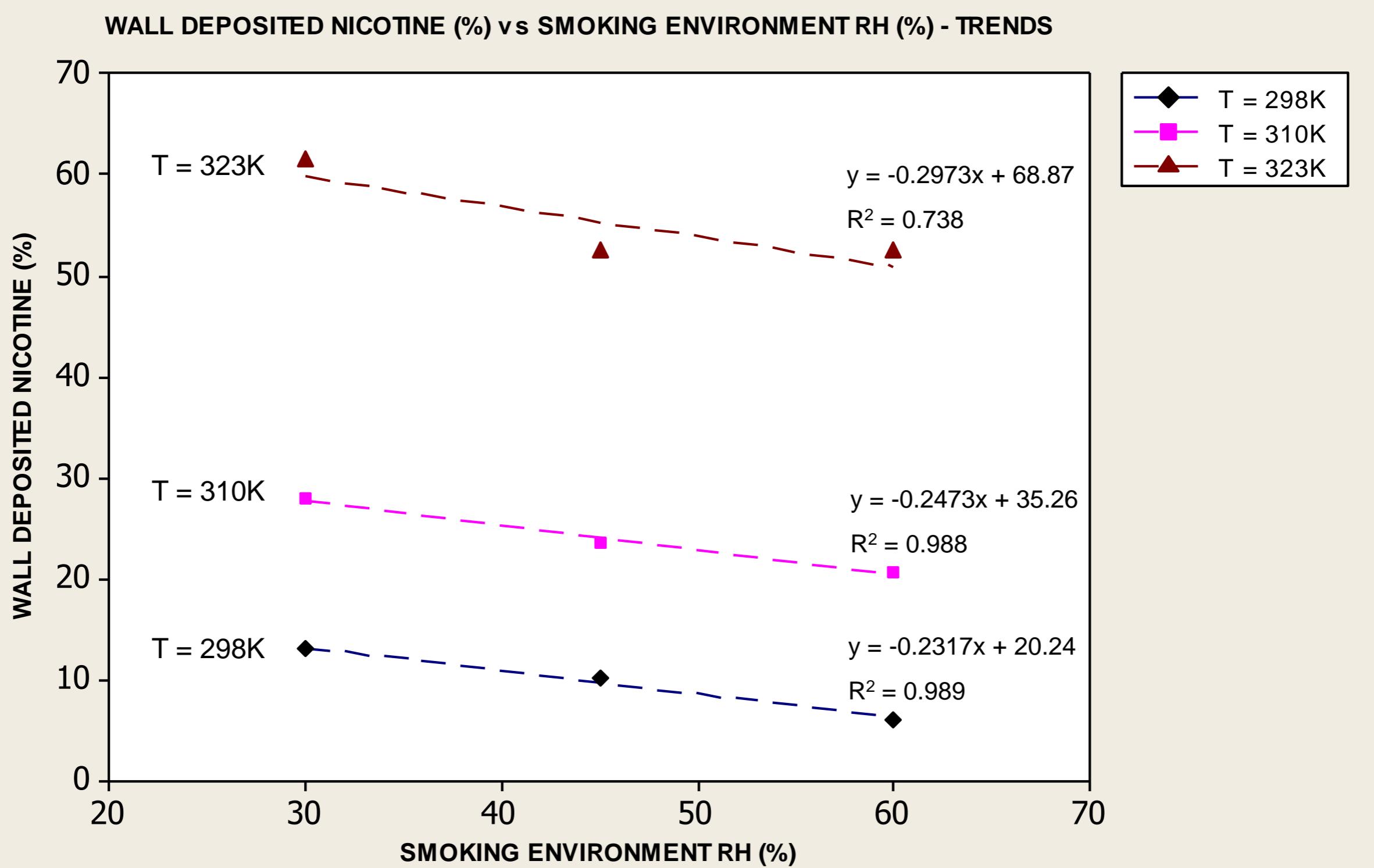


Composite Graph: T = 310K

RH 30%, 45%, 60%

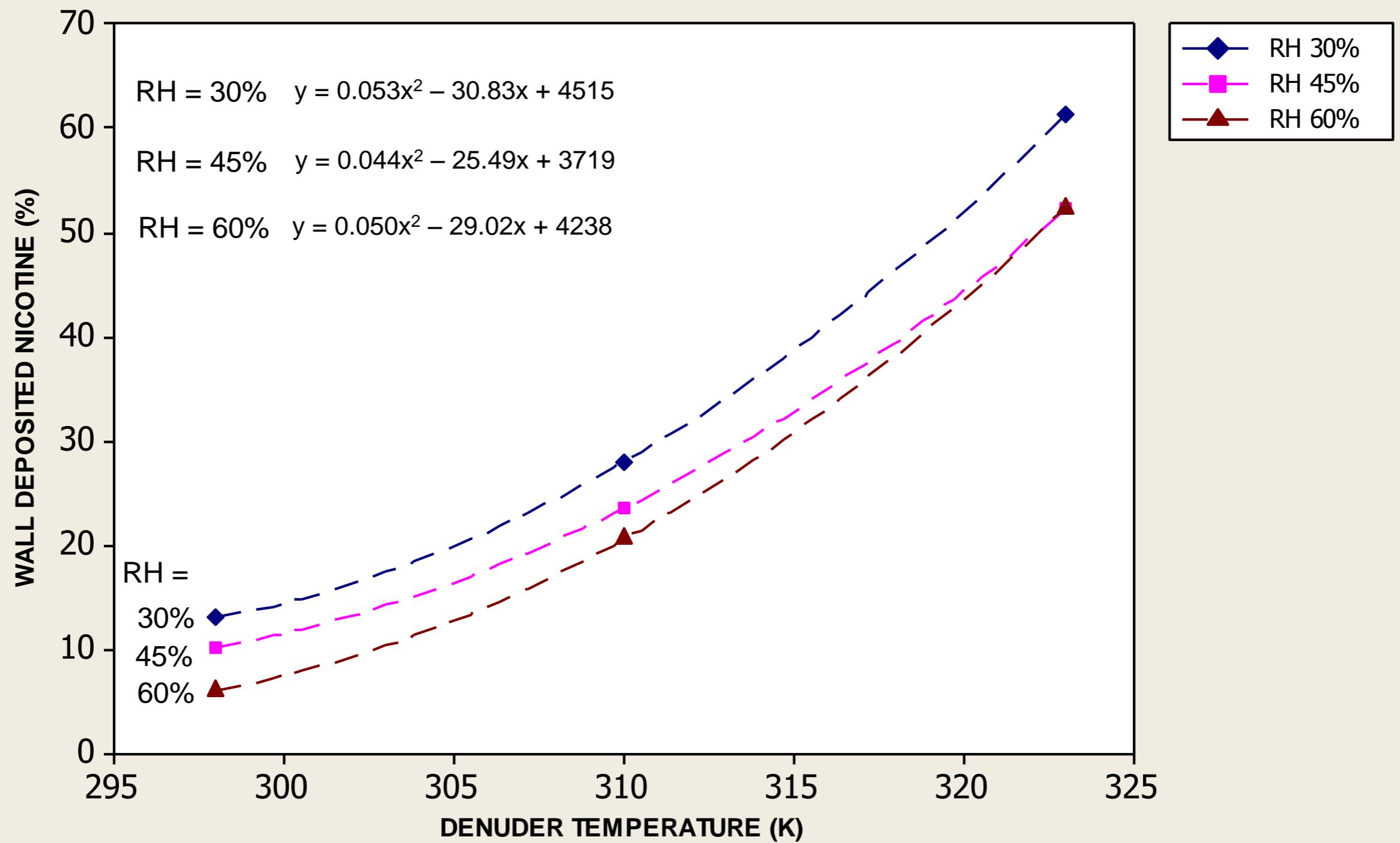


DENUUDER WALL DEPOSITION TRENDS



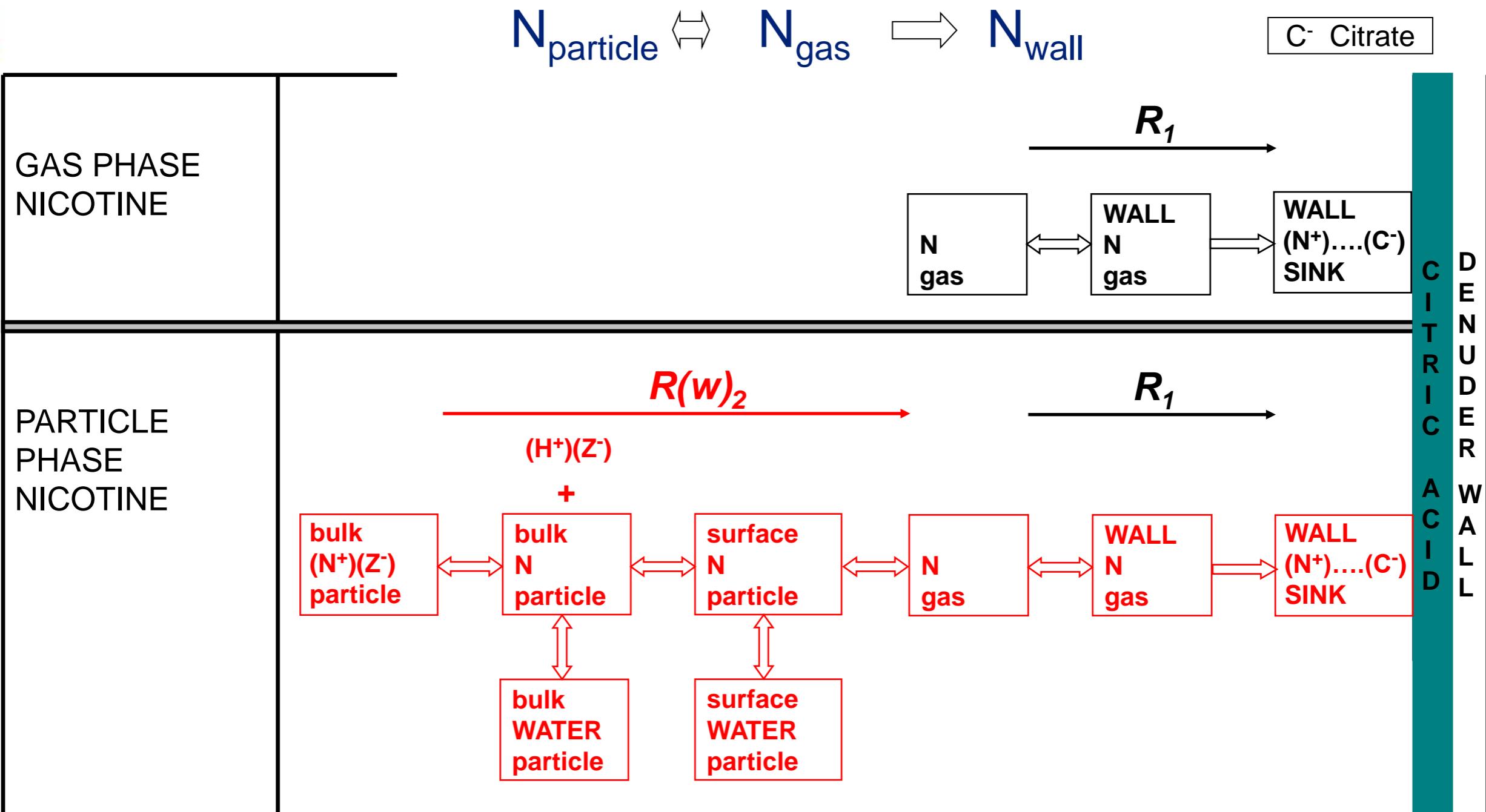
DENUUDER WALL DEPOSITION TRENDS

WALL DEPOSITED NICOTINE (%) vs DENUUDER TEMPERATURE (K) - TRENDS



SMOKE NICOTINE EQUILIBRIA: HUMIDITY EFFECT

Overall Nicotine (N) Equilibria Hypothesis



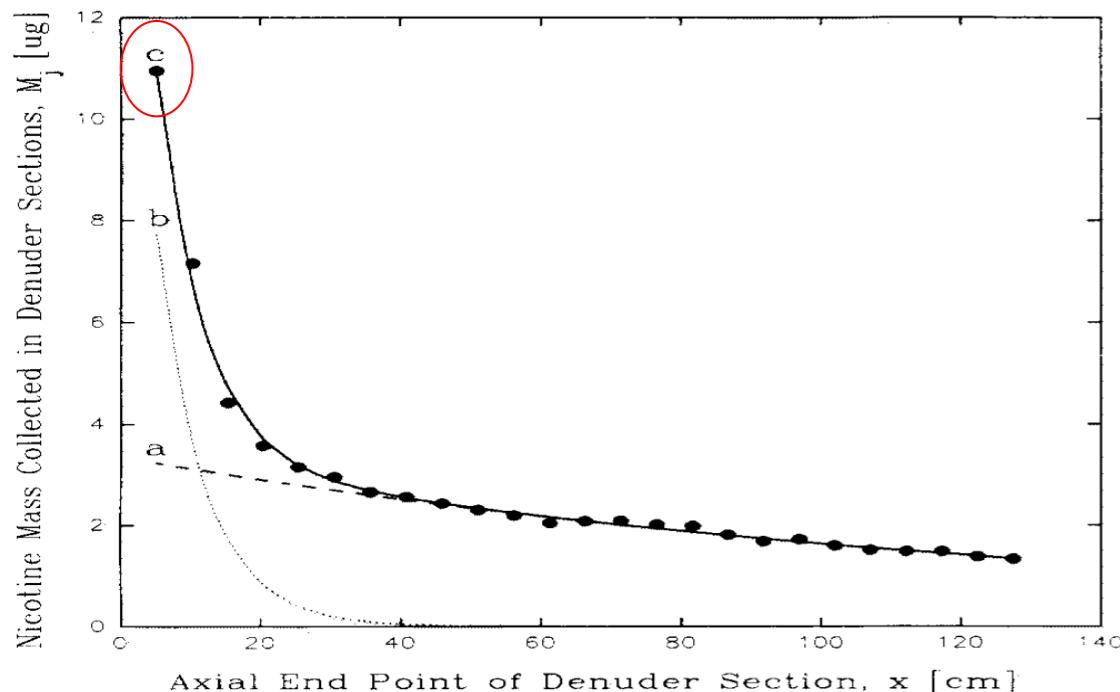
HYPOTHESIS

Physico-chemical principles of water, hygroscopic growth and coagulation influence nicotine release from particles: rate $R(w)_2$

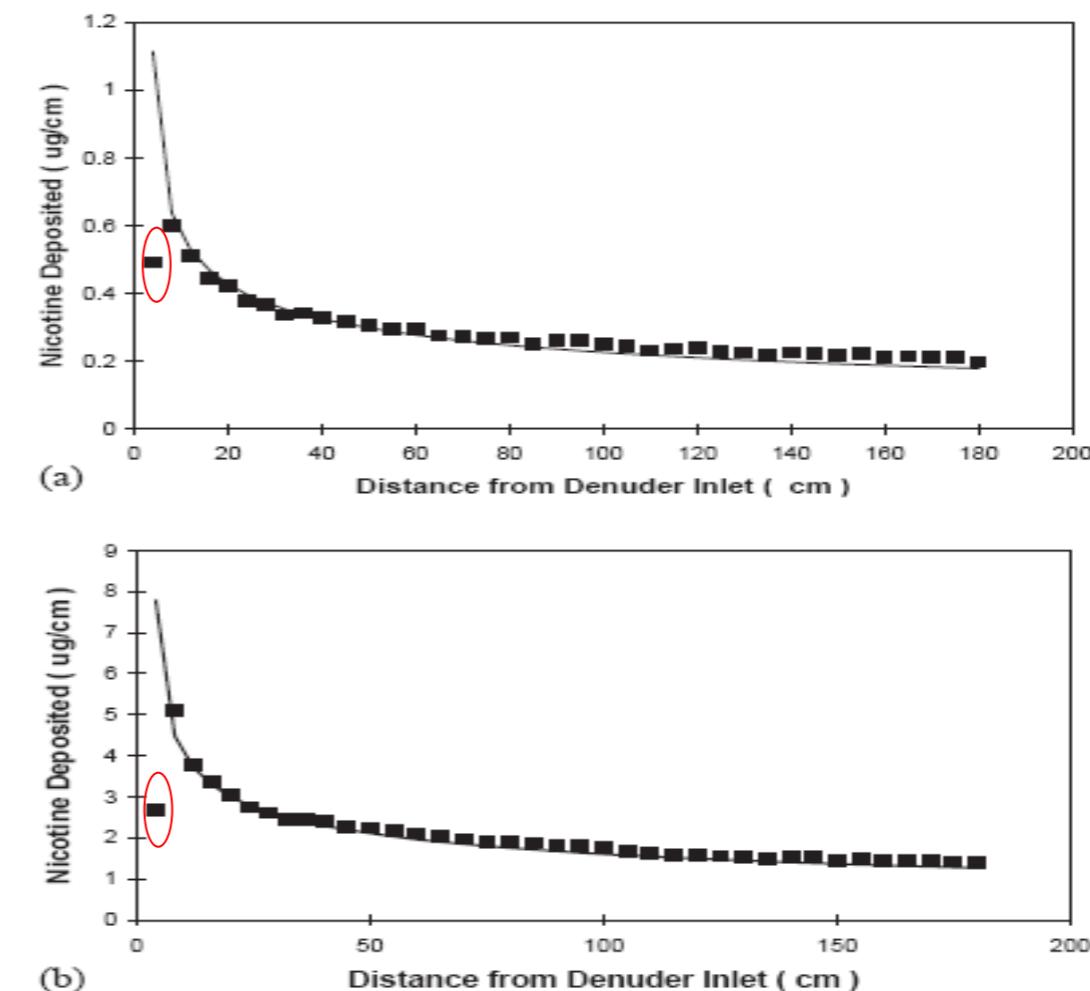
INITIAL GAS PHASE NICOTINE FRACTION

Published Literature

Lewis, D. A., Colbeck, I., Mariner, D. C.,
Analytical Chemistry, **66**, No 20, October 15, 3525 - 3527, (1994)



Lipowicz, P. J., Piadé, J. J.,
Aerosol Science, **35**, 33 - 45, (2004)



Mathematically separates diffusion and evaporation processes from particles; assumes the latter obeys similar alogarithm to the former and additivity

Based on the solution of complex mathematical partial differential equations describing the coupled flow, diffusion and evaporation processes in a denuder tube

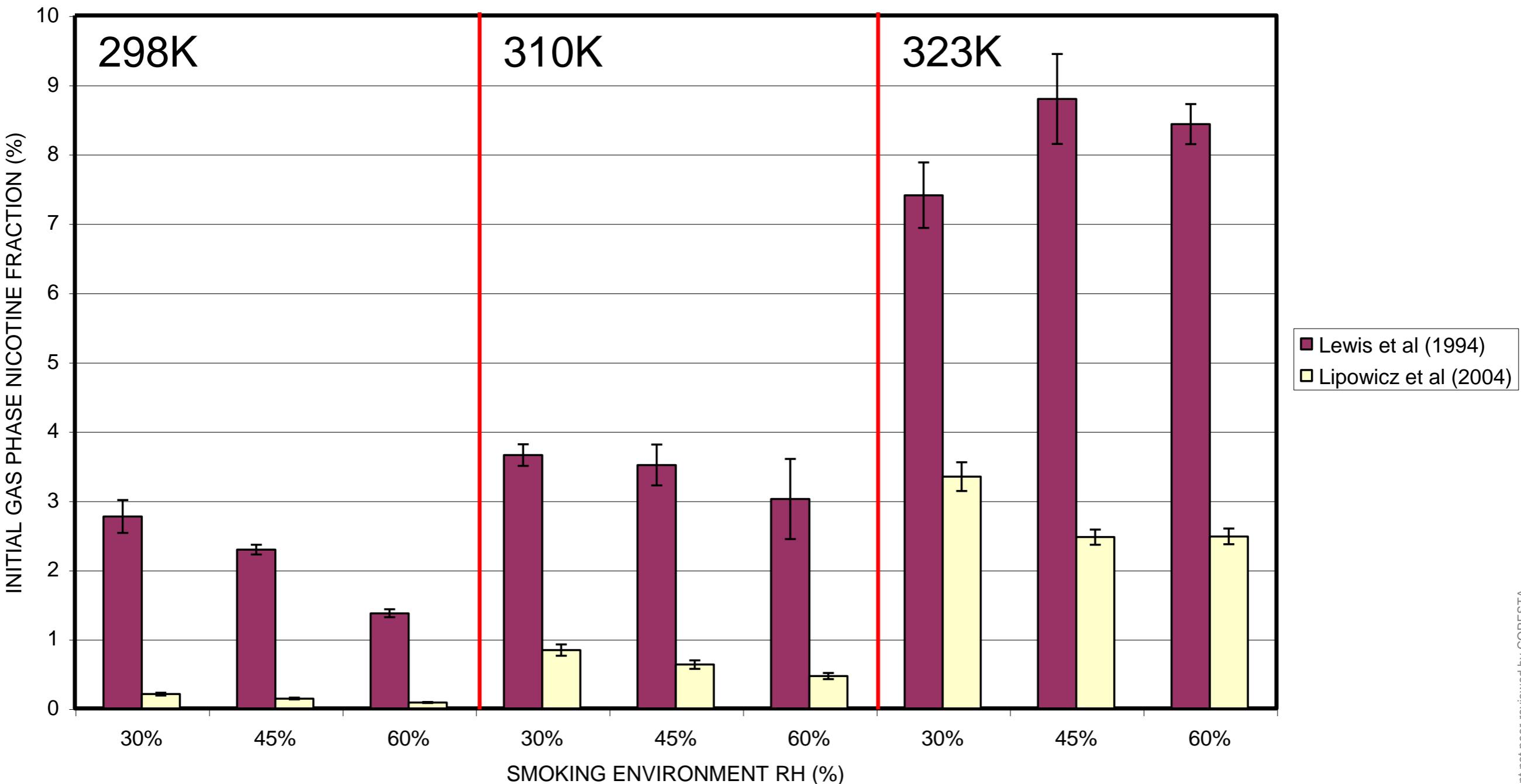
- Lipowicz & Piade: “Application of theory to experimental data shows...the percentage of nicotine initially in the gas phase is about 0.1%, less than previous estimates by an order of magnitude”

Fig (a): Lipowicz analysis - 0.115% gas phase nicotine

Lewis et al analysis – 1.9% gas phase nicotine

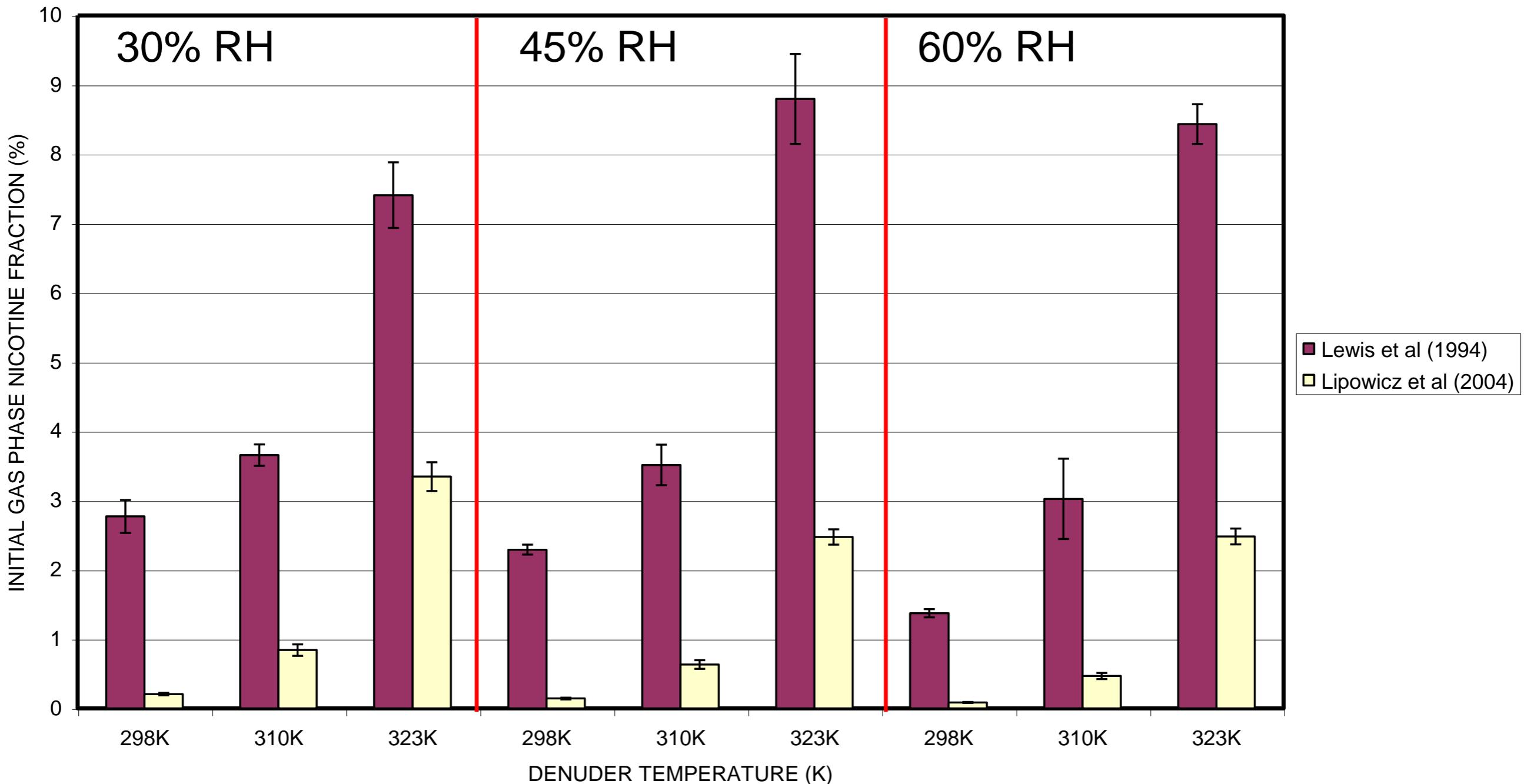
INITIAL GAS PHASE NICOTINE FRACTION: MODELS

COMPARATIVE MODELS: INITIAL GAS PHASE NICOTINE FRACTION (%) ESTIMATION -
SMOKING ENVIRONMENT RH and DENUDER TEMPERATURE EFFECTS



INITIAL GAS PHASE NICOTINE FRACTION: MODELS

COMPARATIVE MODELS: INITIAL GAS PHASE NICOTINE FRACTION (%) ESTIMATION -
SMOKING ENVIRONMENT RH and DENUDER TEMPERATURE EFFECTS



SUMMARY AND CONCLUSIONS

- Advanced denuder system
 - range of operational conditions, RH/temperature/flow/smoke dilution
 - performance verified
- Nicotine particle/gas phase distributions studied
- Gas phase nicotine decreased as:
 - smoking environment RH increased
 - denuder temperature decreased
- First point: anomaly
 - can be continuous or discontinuous re trend line
 - behaviour recreated via tip ventilation open vs closed
- Initial gas phase fraction of nicotine
 - difference depending on calculation model
- Future work:
 - first point anomaly: resolution
 - RH/denuder temperature studies
 - model development

This presentation is available on bat-science.com